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NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species

Bonnie J. McBride, Michael J. Zehe, and Sanford Gordon
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September 2002

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In Memoriam

Sanford Gordon
1920 to 2001

This report is dedicated to the memory of Sanford Gordon, who pioneered the application of computers for calculating thermodynamic properties and for using these properties to model the behavior of reacting systems.

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NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species

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Summary

This report documents the library of thermodynamic data used with the NASA Glenn computer program CEA (Chemical Equilibrium with Applications). This library, containing data for over 2000 solid, liquid, and gaseous chemical species for temperatures ranging from 200 to 20 000 K, is available for use with other computer codes as well. The data are expressed as least-squares coefficients to a seven-term functional form for $C_p^o(T)/R$ with integration constants for $H^o(T)/RT$ and $S^o(T)/R$. The NASA Glenn computer program PAC (Properties and Coefficients) was used to calculate thermodynamic functions and to generate the least-squares coefficients. PAC input was taken from a variety of sources. A complete listing of the database is given along with a summary of thermodynamic properties at 0 and 298.15 K.

Introduction

Thermodynamic data for individual species are required in many applications involving chemical reactions. For over 50 years the NASA Lewis (now Glenn) Research Center has been compiling and disseminating thermodynamic data for use in its chemical equilibrium programs. These data, widely used by the thermodynamic community, have grown from 42 species to the current 2000.

For calculation purposes, the use of thermodynamic data in the form of simple empirical equations has some obvious advantages. First, it makes tabular interpolations unnecessary; second, it permits analytical integrations; and, third, it condenses all the tabulated information into a few constants that accurately reproduce the many thermodynamic data points.

Earlier versions of the NASA Lewis chemical equilibrium computer programs (Gordon et al., 1971, Svehla et al., 1973, Gordon et al., 1976, Gordon et al., 1984, Gordon et al., 1988, and McBride et al., 1994) used a fourth-order polynomial as an empirical representation of $C_p^o(T)/R$ over a temperature range of 300 to 5000 K. The final library of data using this form contained 1130 species documented in NASA TM–4513 (McBride et al., 1993b). For the data in the current report, two terms involving T^{-1} and T^{-2} were added for more accuracy over wider temperature ranges.

A new format was selected that would not only accommodate these two new constants but also allow for revisions and expansions in the future. Features of the new format and how they were used in this report are as follows:

(1) Up to eight constants can be used in the empirical equation for $C_p^o(T)/R$. Only seven were used for the data reported here.

(2) Variable temperature intervals can be used. This new feature was helpful in obtaining good fits for condensed species, which often have irregularly shaped curves and variable transition points. However, standard temperature intervals were used for gases. With a few exceptions, fixed intervals fit the thermodynamic functions for gases accurately.

(3) There is space for comments and references.

(4) The chemical formula may now contain up to five unique atoms. The previous format allowed for only four atoms.

(5) Variable and noninteger temperature exponents are now permitted in the empirical equation for $C_p^o(T)/R$. We used the exponents –2, –1, 0, 1, 2, 3, and 4.

(6) The new format is easier to read. For convenience, values are also given for the molecular weight, heat of formation, and $H^o(298.15) - H^o(0)$.

All symbols used in this report are listed and defined in appendix A. Appendix B contains tables summarizing the thermodynamic data at 0 and 298.15 K. Appendix C gives a description of the particular format used for the database, and appendix D is a complete listing of the NASA Glenn coefficient data as of the date of this report.

The data for individual species are updated as new measurements and estimates appear in the literature. The database is distributed freely via a request form on the internet at http://www.grc.nasa.gov/WWW/CEAWeb/.

Standard States, Reference States, and Fundamental Constants

The symbols and definitions follow the recommendations of Cox (1982). All data in this report are for species in their standard state at the specified temperature. For gases, this is the ideal gas at the standard pressure, 1 bar. For condensed species, the standard state is the pure crystalline or liquid substance at the standard pressure, 1 atm. All thermodynamic properties are molar quantities.

In order for heats of formation to be unambiguously related to specific reactions, a set of reference states must be specified for the chemical elements. The reference state of the elements is generally taken to be the thermodynamically stable state at 298.15 K. For those elements which are gases at 298.15 K and 1 bar, the reference state is taken as gaseous over the entire temperature range. For species that are condensed at 298.15 K, the entire range is taken to be condensed with transitions between various phases. In appendix D, these reference species have either 'Ref-elm' or 'Ref-species' following their name.

Fundamental constants were taken from Cohen et al. (1987). The values used for the molar gas constant R, the Sackur-Tetrode constant S_o/R, the second radiation constant c_2, and the electron mass m_e are given in the symbol list in appendix A. Some thermodynamic functions taken from the literature were calculated using values of R and Sackur-Tetrode constants different from those selected for this report. In these cases, corrections were made to the thermodynamic functions to adjust for the differences. Corrections were made to entropy and Gibbs energy values that had been previously calculated using 1 atm for the standard state pressure rather than 1 bar.

The atomic weights were taken from Coplen (1996). These weights are given in atomic mass units, u, based on $^{12}C = 12$ u.

Empirical Equations for Fitting Thermodynamic Functions

Thermodynamic data for many individual species can be conveniently stored for use with computer programs in the form of coefficients associated with equations that reproduce the data. The following dimensionless form was chosen for this report:

$$C_p^o(T)/R = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4 \quad (1)$$

Enthalpy and entropy are obtained by integrating $C_p^o(T)$ and $C_p^o(T)/T$, respectively, with respect to T:

$$H^o(T)/RT = -a_1T^{-2} + a_2 lnT/T + a_3 + a_4T/2 + a_5T^2/3 + a_6T^3/4 + a_7T^4/5 + b_1/T \quad (2)$$

$$S^o(T)/R = -a_1T^{-2}/2 - a_2T^{-1} + a_3 lnT + a_4T + a_5T^2/2 + a_6T^3/3 + a_7T^4/4 + b_2 \quad (3)$$

where b_1 and b_2 are integration constants. These equations have been found to accurately reproduce the thermodynamic quantities over a wide temperature range.

Assigned Enthalpy Values

For each species, heats of formation (and, when applicable, heats of transition) were combined with sensible heats, $H^o(T) - H^o(298.15)$, to give the assigned enthalpies, $H^o(T)$. By definition

$$H^o(T) \equiv H^o(298.15) + [H^o(T) - H^o(298.15)] \quad (4)$$

We arbitrarily assign $H^o(298.15) = \Delta_f H^o(298.15)$. The above equation then becomes

$$H^o(T) = \Delta_f H^o(298.15) + [H^o(T) - H^o(298.15)] \quad (5)$$

In general, $H^o(T)$ will not equal $\Delta_f H^o(T)$ except at 298.15 K. Similarly, for the $H^o(0)$ values listed in tables B1 and B2 in appendix B,

$$H^o(0) = \Delta_f H^o(298.15) - [H^o(298.15) - H^o(0)] \quad (6)$$

All reference elements and the reference species electron gas have assigned enthalpy values, $H^o(298.15)$, equal to zero.

Assigned enthalpies for reactants are listed in table B3 in appendix B. For noncryogenic reactants, assigned enthalpies are given at 298.15 K. For cryogenic liquids, assigned enthalpies are given at their boiling points

instead of 298.15 K. These are obtained by subtracting the following values from the heat of formation of the gas at 298.15 K: (1) the sensible heat of the ideal gas at 298.15 K relative to the boiling point, (2) the relative enthalpy of the ideal gas to the real gas at the boiling point, and (3) the heat of vaporization at the boiling point.

Heats of Formation and Equilibrium Constants

At any temperature, values of $\Delta_f H^o$ and $\log_{10} K$ may be calculated for the formation of a species from its constituent elements in their assigned reference states. The following is an example of how these properties can be calculated for CO(g) at 1000 K:

$$\Delta_f H^o(1000) = H^o(1000)\ \mathrm{CO(g)} - H^o(1000)\mathrm{C(graphite)} - \tfrac{1}{2}H^o(1000)\ \mathrm{O_2(g)} \quad (7)$$

$$\Delta_f G^o(1000) = G^o(1000)\ \mathrm{CO(g)} - G^o(1000)\mathrm{C(graphite)} - \tfrac{1}{2}G^o(1000)\ \mathrm{O_2(g)} \quad (8)$$

By definition,

$$\log_{10} K \equiv -\Delta_f G^o(T)/(2.3025851\ RT) \quad (9)$$

Properties and Coefficients (PAC) Programs

The NASA Glenn computer program PAC99 was used to convert molecular constants and thermodynamic data into the coefficient form described in appendix C. PAC99 is the latest in a series of FORTRAN programs that generate data in the format required by CEA. It is an expanded version of PAC91 (McBride et al., 1992). The expansion includes new techniques for calculating properties for atomic species (Gordon et al., 1999), increased dimensions for larger molecules, and the capacity to use more parameters in internal rotor calculations. The following sections discuss the tasks performed by this program.

Thermodynamic Properties

Thermodynamic properties may be read in either as thermodynamic functions or as coefficients. A method for extrapolating these data to higher temperatures is provided. For gases, PAC99 provides several methods for calculating thermodynamic functions from molecular data.

The calculation methods used for monatomic gases are outlined in Gordon et al. (1999). For polyatomic species, six closed-form calculation methods are available (McBride et al., 1992). All were used in this report. All use a rigid-rotor harmonic-oscillator base with corrections for anharmonicities, vibration-rotation interactions, rotational stretching, low-temperature quantum rotation, Fermi and Darling-Dennison resonance, and internal rotation. The Darling-Dennison resonance and some low-temperature quantum corrections (Gurvich et al., 1989) have been added since PAC91. The internal rotor calculations were also expanded to use more potential and rotational constants (Lewis et al., 1972, and Zeleznik, 2002). Equilibrium mixtures of isomers were calculated by summing the partition functions for each conformer. PAC99 calculates tables of thermodynamic functions including $\Delta_f H^o$ and $\log_{10} K$ with an option to do a least-squares fit of the data.

Least-Squares Fit

Most coefficients in equations (1) to (3) were obtained using the least-squares fit feature in PAC99. For gases, the temperature ranges for these fits are split into three fixed intervals: 200 to 1000 K (298.15 to 1000 K for ions), 1000 to 6000 K, and for some simple molecules, 6000 to 20 000 K. For condensed species, the temperature ranges are variable, with each phase having its own set of coefficients. The fits were subject to the following constraints:

(1) An exact fit at 298.15 K.

(2) Coefficients for two contiguous intervals yield the same functional values at the common point.

(3) The difference in Gibbs energy is zero between condensed phases.

(4) Generally $C_p^o(T)/R$, $[H^o(T) - H^o(0)]/RT$, and $S^o(T)$ were fit simultaneously as suggested by Zeleznik et al. (1961). However, this method was not used for monatomic species, where electronic levels were truncated with a temperature-dependent cutoff technique (Gordon et al., 1999). For these cases, the least-squares fit was on $C_p^o(T)/R$ only.

Generally for intervals where $C_p^o(T)/R$ is constant, a least-squares fit was not done.

Data Sources

Each species within the coefficient data file (app. D) contains abbreviated references to the data used to generate those coefficients. Complete reference citations, ordered by first author's last name and year, are listed at the end of this report.

Heats of formation were often obtained indirectly from other values (e.g., dissociation energies). This required the use of additional thermodynamic data. Generally, the supporting data were taken from the NASA database, otherwise the references are indicated.

For condensed species, either thermodynamic functions or fitted coefficients were taken directly from the references listed. For most gases the functions were calculated with the PAC99 program using molecular data from the cited references and any of several calculation techniques. However, for diatomic gases most of the functions were taken directly from the Gurvich references because they used a direct summation method not currently part of PAC99. If molecular constants for excited electronic states of diatomic and polyatomic gases were not available in the source reference, they were taken from another electronic state, usually the ground state.

Calculation techniques for monatomic species are described in Gordon et al. (1999). When thermodynamic functions for a gas were taken directly from the literature and were not given to high enough temperatures (e.g., 6000 or 20 000 K), they were extrapolated by the method described in Wilhoit (1975). Extrapolations were done in order to provide reasonable values outside the temperature range of the original data, which is important when CEA iterates on T. During the iteration, T may be temporarily out of range of the original data, resulting in thermodynamic properties so inaccurate that convergence is impossible.

Thermodynamic Properties at 0 and 298.15 K

A summary of the thermodynamic properties at 0 and 298.15 K is given in appendix B. There are three tables:

Table B1.—Thermodynamic Properties for Gases at 0 and 298.15 K

Table B2.—Thermodynamic Properties for Condensed Species at 0 and 298.15 K

Table B3.—Assigned Enthalpies for Species That Are Used in CEA as Reactants Only

Note that reactants-only species with coefficients appear not only in table B3 but also in table B1 or B2. The thermodynamic quantities at 298.15 K were calculated from the coefficients. Since the least-squares fits are constrained to fit these values, the listed quantities match the source values. The third table lists assigned enthalpies and associated temperatures, molecular weights, and stoichiometric coefficients for species in the reactant-only class. No other thermodynamic quantities are listed in this table because coefficients are not available for most of the species.

Thermodynamic Coefficients Data

Appendix D lists the thermodynamic data as distributed in a file called thermo.inp. Appendix C discusses the format of this file. It shows the exact placement of names, references and comments, reference-date codes, chemical formula, molecular weights, heats of formation, $H^o(T) - H^o(0)$ values, temperature ranges, number of temperature intervals, phase code, and coefficients.

The following sections contain general comments on species names, data order, and miscellaneous information useful in interpreting the database. Each line of data is referred to as a record.

Species Names

The first 15 characters in the first record are reserved for the species name, usually the chemical formula. Longer names are often truncated. The letter "l," which is normally lowercase, has been replaced with uppercase "*L*" to avoid confusion with the number "1." Condensed phases designated as α, β, γ, or δ are called *a*, *b*, *c*, or *d* because FORTRAN does not allow Greek letters. Similarly, numbers normally shown as subscripts are printed on the main line for the same reason.

References

References and comments follow the species name in record 1. References are usually depicted by the first author's last name and the year of publication. An exception is for the TRC (Thermodynamic Research Center) looseleaf tables, where page and table date are used. Comments are abbreviated to fit the space available. When the heat of formation is taken from a separate reference, it is indicated as "Hf:". Reference elements

or reference species used for heats of formation are indicated by "Ref-Elm." or "Ref-Species."

Species Order

The data are divided into three categories and are listed in the following order:

(1) Gases used in CEA as possible products and reactants (pp. 45–210)

(2) Condensed species used in CEA as possible products and reactants (pp. 210–276)

(3) Species that may be used only as reactants in CEA (e.g., air or Jet-A) (pp. 276–280)

Within the first two categories, the species are listed alphabetically according to the chemical formula given on the second record. The reactants-only set is listed alphabetically by name. This set is separated from the first two by a single record "END PRODUCTS" (see p. 276).

For condensed species with multiple phases, individual phases are listed in increasing order according to their temperature ranges. Consecutive phases are numbered consecutively starting with "1" in column 52 in record 2. See appendix C.

Reference-Date Codes

Record 2 contains a six-character code designating a reference and date as defined at the beginning of appendix D. The alphabetic part of the code represents a large compilation of data (e.g., "j" for JANAF or "g" for Glenn Research Center). The "g" was used if the PAC99 input data either (1) came from mixed sources, (2) came from a source not coded, (3) were molecular constants where no thermodynamic functions were given in the source, or (4) were molecular constants with a calculation method differing from the method used by the source.

Temperature Ranges

For nonionic gases, the temperature range of the fitted data is either 200 to 6000 K, or 200 to 20 000 K. For ionic gases, the starting temperature is 298.15 K. Only the electron gas, monatomic species, and simple molecules (e.g., CO, CO_2, N_2, NO, and O^+) have been fitted to 20 000 K. For gases, there is a breakpoint in the fit at 1000 K. For gases fitted to 20 000 K, there is an additional breakpoint at 6000 K. Each temperature range is listed in the record preceding the corresponding coefficients. For condensed species, the temperature ranges and breakpoints are set according to the data and accuracy of the fits.

Using the Coefficients to Obtain Thermodynamic Functions

The NASA Glenn database can be used to obtain listings of thermodynamic functions, either interactively online with the Properties From Coefficients (PFC) computer program or by use of the Coefficients and Properties (CAP) computer program (Zehe et al., 2001).

The PFC interactive program provides a Periodic Table of the Elements from which the user selects constituent atoms for the species to be tabulated. PFC presents a list of all species in the database containing those elements. The user selects the species of interest and the temperature schedule to be used. PFC lists the current NASA coefficients for those species and uses them to create a table of $C_p^o(T)$, $H^o(T) - H^o(298.15)$, $S^o(T)$, $-[G^o(T) - H^o(T)]/T$, $H^o(T)$, $\Delta H_f{}^o(T)$, and log $K(T)$ at each temperature in the schedule. Data are also listed for 0 K, 298.15 K, and for all phase changes within the temperature schedule. PFC can be accessed directly at http:///cea.grc.nasa.gov or from the CEA Web site http://www.grc.nasa.gov/WWW/CEAWeb/ with the selection "Get Properties from NASA Coefficients (PFC)."

The CAP program allows users to tabulate thermodynamic functions from the NASA Glenn coefficients without being connected to the Internet. Thermodynamic functions may be tabulated in SI units, in chemical units (calories and kelvin), or in "engineering" units (Btu/lb-mol and Btu/lb-mol-°R). An option allows the user to generate a file listing temperatures and thermodynamic functions in column format for easy plotting. The program is described in NASA/TP—2001-210959 (Zehe et al., 2001). CAP and the NASA Glenn database are available via a request form at the CEA Web site http://www.grc.nasa.gov/WWW/CEAWeb/.

National Aeronautics and Space Administration
John H. Glenn Research Center at Lewis Field
Cleveland, Ohio 44135, April 11, 2002

Appendix A
Symbols

a_i $(i = 1, 7)$	temperature coefficients in eqs. (1), (2), and (3)
b_1, b_2	integration constants defined by eqs. (2) and (3)
$C_p^o(T)$	molar heat capacity at constant pressure at temperature T for standard state, eq. (1)
c_2	second radiation constant, 1.438769 cm-K
$G^o(T)$	either $[G^o(T) - H^o(0)] + H^o(0)$ or $[G^o(T) - H^o(298.15)] + H^o(298.15)$
$G^o(T) - H^o(0)$	molar Gibbs energy at temperature T relative to enthalpy at 0 K for standard state
$G^o(T) - H^o(298.15)$	molar Gibbs energy at temperature T relative to enthalpy at 298.15 K for standard state
$H^o(T)$	either $[H^o(T) - H^o(0)] + H^o(0)$ or $[H^o(T) - H^o(298.15)] + H^o(298.15)$
$H^o(T) - H^o(0)$	molar enthalpy at temperature T relative to molar enthalpy at 0 K for standard state
$H^o(T) - H^o(298.15)$	molar enthalpy at temperature T relative to molar enthalpy at 298.15 K for standard state
$H^o(0)$	chemical energy (molar enthalpy) at 0 K for standard state
$H^o(298.15)$	assigned molar enthalpy at 298.15 K for standard state (equals $\Delta_f H^o(298.15)$)
K	equilibrium constant
m_e	electron mass, 0.000548579903 u
R	universal gas constant, 8.314510 J/(mol-K)
$S^o(T)$	entropy at temperature T for standard state
S_o/R	Sackur-Tetrode constant for $p_o = 1$ bar, -1.151693
T	temperature, K
$\Delta_f G^o(T)$	molar Gibbs energy of formation of a substance at temperature T from its reference species in their standard state
$\Delta_f H^o(T)$	molar enthalpy of formation (heat of formation) of a substance at temperature T from its reference species in their standard state

Appendix B
Thermodynamic Properties at 0 and 298.15 K

This appendix contains three tables summarizing the properties of the species in thermo.inp (app. D) at 0 and 298.15 K. Table B1 is for all gaseous species that have coefficients including those used in the NASA program CEA (Chemical Equilibrium with Applications) for reactants-only species. Table B2 lists data for all condensed species. Table B3 summarizes information for all the reactants-only species whether or not they have coefficients.

For cryogenic liquids in this last table, assigned enthalpies $H^o(T)$ are given at their boiling points rather than 298.15 K. For more details on assigned enthalpies see the section "Assigned Enthalpy Values."

TABLE B1.—THERMODYNAMIC PROPERTIES FOR GASES AT 0 AND 298.15 K

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
e-	5.4858-04	-6.197	-6.197	0.000	20.786	6.197	20.979
Ag	107.86820	278.703	284.448	284.900	20.786	6.197	172.998
Ag+	107.86765	1015.896	1015.444	1022.094	20.792	6.198	167.236
Ag-	107.86875	146.881	158.824	153.079	20.786	6.197	167.235
AL	26.98154	323.081	327.621	330.000	21.391	6.919	164.555
AL+	26.98099	906.818	905.160	913.015	20.786	6.197	149.952
AL-	26.98209	274.334	285.071	281.090	20.960	6.756	168.137
ALBr	106.88554	4.754	21.554	14.325	35.618	9.571	239.635
ALBr2	186.78954	-154.060	-125.000	-140.662	53.256	13.398	312.236
ALBr3	266.69354	-428.420	-387.100	-410.477	75.372	17.943	348.026
ALC	38.99224	673.225	678.819	682.284	33.218	9.058	225.918
ALC2	51.00294	663.353	670.000	675.616	47.818	12.263	252.941
ALCL	62.43424	-60.331	-51.200	-51.007	34.661	9.323	227.961
ALCL+	62.43369	852.695	855.628	861.849	33.794	9.154	232.190
ALCL2	97.88694	-253.721	-240.000	-240.874	51.566	12.847	290.374
ALCL3	133.33964	-601.080	-582.768	-584.679	71.537	16.401	313.089
ALF	45.97994	-272.953	-264.000	-264.060	31.937	8.892	215.162
ALF+	45.97939	683.421	686.176	692.234	31.155	8.813	220.068
ALFCL	81.43264	-448.543	-435.000	-436.410	48.267	12.133	282.721
ALFCL2	116.88534	-807.134	-789.000	-791.395	68.808	15.738	311.383
ALF2	64.97834	-643.365	-630.000	-631.764	45.418	11.601	264.924
ALF2-	64.97889	-864.563	-845.000	-853.231	44.746	11.332	257.271
ALF2CL	100.43104	-1013.956	-996.000	-999.128	65.546	14.828	298.135
ALF3	83.97675	-1223.321	-1205.543	-1209.277	62.199	14.044	276.674
ALF4-	102.97570	-1968.388	-1940.000	-1951.601	80.986	16.787	293.563
ALH	27.98948	240.583	249.357	249.251	29.371	8.668	187.863
ALHCL	63.44218	-0.365	13.000	10.522	42.023	10.887	257.237
ALHCL2	98.89488	-364.955	-347.000	-351.279	60.517	13.676	288.762
ALHF	46.98788	-193.187	-180.000	-182.614	39.732	10.572	245.469
ALHFCL	82.44058	-567.777	-550.000	-555.245	56.969	12.533	278.249
ALHF2	65.98628	-777.599	-760.000	-765.299	53.676	12.300	263.716
ALH2	28.99742	266.684	279.692	276.775	35.773	10.091	213.316
ALH2CL	64.45012	-117.599	-100.000	-106.345	47.528	11.253	251.100
ALH2F	47.99582	-327.421	-310.000	-316.656	44.221	10.765	238.744
ALH3	30.00536	118.486	135.728	128.896	40.057	10.411	206.579

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
ALI	153.88601	57.644	68.782	67.395	36.135	9.751	247.840
ALI2	280.79048	-47.736	-30.000	-33.813	54.635	13.923	328.828
ALI3	407.69495	-210.334	-186.000	-191.330	77.474	19.004	373.832
ALN	40.98828	429.564	438.439	438.829	32.417	9.265	228.437
ALO	42.98094	58.531	67.411	67.319	30.884	8.788	218.389
ALO+	42.98039	983.903	986.586	992.993	33.135	9.090	230.978
ALO-	42.98149	-281.666	-266.589	-272.922	30.335	8.745	211.945
ALOCL	78.43364	-313.471	-300.000	-301.565	50.368	11.906	252.377
ALOCL2	113.88634	-418.061	-400.000	-402.309	68.896	15.752	316.893
ALOF	61.97934	-583.293	-570.000	-572.290	46.787	11.003	238.965
ALOF2	80.97774	-787.705	-770.000	-773.650	62.253	14.055	291.335
ALOF2-	80.97829	-986.367	-962.464	-972.290	62.593	14.077	284.874
ALOH	43.98888	-203.114	-190.000	-192.762	43.512	10.352	222.643
ALOHCL	79.44158	-387.705	-370.000	-373.786	57.901	13.919	294.387
ALOHCL2	114.89428	-742.295	-720.000	-725.145	77.819	17.150	325.075
ALOHF	62.98728	-587.527	-570.000	-574.212	54.626	13.315	282.240
ALOHF2	81.98568	-1156.939	-1135.000	-1141.511	70.799	15.428	299.541
ALO2	58.98034	-52.020	-38.799	-38.658	51.661	13.362	269.317
ALO2-	58.98089	-463.217	-443.799	-452.572	46.063	10.645	229.783
AL(OH)2	60.99622	-521.688	-500.000	-507.661	62.980	14.028	284.406
AL(OH)2CL	96.44892	-876.279	-850.000	-859.057	82.994	17.222	316.305
AL(OH)2F	79.99462	-1086.101	-1060.000	-1069.629	79.532	16.472	304.655
AL(OH)3	78.00356	-1030.262	-1000.000	-1012.668	87.249	17.595	301.541
ALS	59.04754	223.594	232.546	232.682	33.405	9.088	230.619
ALS2	91.11354	234.107	247.471	248.535	56.557	14.429	294.462
AL2	53.96308	491.163	500.243	501.302	37.055	10.139	243.842
AL2Br6	533.38708	-980.640	-898.000	-942.423	167.510	38.217	537.155
AL2C2	77.98448	528.813	540.000	544.978	67.665	16.165	284.603
AL2CL6	266.67928	-1331.023	-1294.400	-1296.876	159.150	34.147	470.448
AL2F6	167.95350	-2658.555	-2623.000	-2632.491	133.312	26.064	385.487
AL2I6	815.38990	-528.668	-480.000	-487.747	171.922	40.921	589.636
AL2O	69.96248	-161.388	-147.968	-148.611	51.978	12.777	253.135
AL2O+	69.96193	635.989	643.212	648.970	52.898	12.981	260.663
AL2O2	85.96188	-418.938	-401.178	-403.096	68.122	15.843	288.044
AL2O2+	85.96133	542.464	554.026	557.439	68.924	14.975	289.704
AL2O3	101.96128	-566.489	-544.388	-546.891	86.990	19.598	316.662
AL2S	86.02908	206.675	220.167	220.679	56.379	14.004	271.338
AL2S2	118.09508	117.188	135.092	135.287	75.938	18.100	320.299
Ar	39.94800	-6.197	-6.197	0.000	20.786	6.197	154.847
Ar+	39.94745	1520.572	1520.572	1526.778	20.984	6.206	166.406
B	10.81100	569.283	570.497	575.599	20.797	6.316	153.438
B+	10.81045	1376.118	1371.135	1382.316	20.786	6.197	138.545
B-	10.81155	536.359	543.770	542.631	20.788	6.273	156.814
BBr	90.71500	231.955	245.429	240.952	32.787	8.997	224.992
BBr2	170.61900	85.628	111.362	97.829	48.451	12.201	294.539
BBr3	250.52300	-221.003	-183.009	-205.300	67.777	15.703	324.505
BC	22.82170	829.427	831.694	838.162	30.217	8.735	210.103
BC2	34.83240	789.571	792.892	801.259	45.718	11.688	236.684
BCL	46.26370	174.312	180.117	183.173	31.656	8.861	213.244
BCL+	46.26315	1225.420	1225.027	1234.280	31.644	8.860	219.133
BCLOH	63.27104	-246.437	-232.058	-234.005	52.322	12.432	272.255
BCL(OH)2	80.27838	-818.953	-796.000	-805.388	68.307	13.565	285.524
BCL2	81.71640	-72.395	-62.000	-60.881	45.746	11.514	271.202
BCL2+	81.71585	659.467	663.664	672.315	52.975	12.849	257.809
BCL2OH	98.72374	-618.969	-600.000	-604.917	66.824	14.052	296.758

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
BCL3	117.16910	-418.471	-403.485	-404.500	62.556	13.971	289.468
BF	29.80940	-115.627	-110.000	-106.932	29.594	8.695	200.453
BFCL	65.26210	-290.217	-280.000	-279.184	42.820	11.033	264.941
BFCL2	100.71480	-656.231	-641.423	-643.000	58.911	13.231	287.581
BFOH	46.81674	-463.605	-449.404	-451.632	49.233	11.973	260.090
BF(OH)2	63.82408	-1062.775	-1040.000	-1049.890	63.510	12.885	274.274
BF2	48.80781	-510.039	-500.000	-499.427	40.055	10.612	247.133
BF2+	48.80726	311.974	315.816	322.586	44.291	10.612	225.151
BF2-	48.80835	-744.237	-728.000	-733.803	39.436	10.434	240.589
BF2CL	84.26051	-900.324	-885.694	-888.000	54.473	12.324	275.115
BF2OH	65.81515	-1104.613	-1086.000	-1092.217	57.769	12.396	272.590
BF3	67.80621	-1147.651	-1133.200	-1136.000	50.462	11.651	254.429
BF4-	86.80516	-1775.062	-1750.000	-1761.266	67.794	13.796	268.855
BH	11.81894	440.088	445.536	448.727	29.181	8.639	171.836
BHCL	47.27164	131.113	141.152	141.418	38.435	10.305	240.471
BHCL2	82.72434	-263.629	-249.000	-251.884	49.656	11.746	268.244
BHF	30.81734	-86.054	-76.194	-76.012	35.458	10.042	227.969
BHFCL	66.27004	-494.451	-480.000	-483.037	47.771	11.415	263.145
BHF2	49.81575	-750.273	-736.000	-739.614	42.230	10.659	244.323
BH2	12.82688	318.885	328.568	328.909	34.975	10.024	193.685
BH2CL	48.27958	-91.273	-77.000	-80.846	40.345	10.427	234.358
BH2F	31.82528	-334.095	-320.000	-323.957	37.204	10.138	222.022
BH3	13.83482	94.687	108.603	104.747	36.018	10.060	188.251
BH3NH3	30.86538	-127.682	-96.728	-115.000	56.999	12.682	240.883
BH4	14.84276	244.440	262.590	255.210	44.277	10.771	211.994
BH5	15.85070	80.361	102.745	92.934	52.616	12.572	229.549
BI	137.71547	316.845	324.657	325.988	33.731	9.142	233.319
BI2	264.61994	225.408	239.818	238.096	50.294	12.688	311.115
BI3	391.52441	4.467	25.475	21.400	71.027	16.933	350.427
BN	24.81774	565.765	571.314	574.726	29.519	8.961	212.781
BO	26.81040	11.732	17.286	20.406	29.196	8.674	203.468
BO-	26.81095	-286.465	-274.714	-277.791	29.197	8.674	197.683
BOCL	62.26310	-329.145	-319.000	-318.537	45.079	10.608	237.306
BOCL2	97.71580	-374.735	-360.000	-361.566	58.826	13.170	292.296
BOF	45.80880	-602.967	-593.000	-592.978	41.653	9.988	224.981
BOF2	64.80721	-844.379	-830.000	-832.768	50.491	11.611	268.239
BOH	27.81834	-16.788	-7.000	-6.757	35.350	10.032	217.899
BO2	42.80980	-319.894	-310.000	-309.122	43.285	10.772	230.138
BO2-	42.81035	-724.092	-708.000	-714.494	39.147	9.598	215.734
B(OH)2	44.82568	-437.215	-418.853	-425.244	54.191	11.972	259.389
BS	42.87700	264.795	270.421	273.519	30.052	8.724	216.195
BS2	74.94300	50.308	60.346	63.867	55.498	13.560	267.139
B2	21.62200	848.565	850.993	857.371	31.503	8.805	202.064
B2C	33.63270	788.710	792.191	800.433	46.228	11.723	225.242
B2CL4	163.43280	-511.588	-490.798	-490.000	97.997	21.588	371.268
B2F4	97.61561	-1455.681	-1435.603	-1438.000	80.629	17.681	326.206
B2H	22.62994	786.147	792.809	796.262	42.328	10.116	214.282
B2H2	23.63788	444.105	455.001	454.678	48.195	10.573	214.235
B2H3	24.64582	339.134	354.264	351.073	52.523	11.939	236.055
B2H3,db	24.64582	341.497	356.627	353.408	52.473	11.911	232.835
B2H4	25.65376	198.822	218.186	211.162	57.117	12.340	230.385
B2H4,db	25.65376	198.404	217.768	209.932	51.510	11.529	228.028
B2H5	26.66170	242.563	266.161	254.784	58.182	12.221	243.502
B2H5,db	26.66170	263.483	287.081	275.151	53.171	11.668	245.703
B2H6	27.66964	24.668	52.500	36.600	56.643	11.932	232.027

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
B2O	37.62140	181.015	187.783	192.798	47.247	11.783	226.244
B2O2	53.62080	-471.108	-460.000	-457.711	60.269	13.397	249.669
B2O3	69.62020	-849.801	-834.353	-835.382	64.917	14.419	285.902
B2(OH)4	89.65136	-1274.431	-1237.706	-1254.988	105.026	19.443	347.137
B2S	53.68800	609.078	615.918	622.261	52.763	13.183	248.243
B2S2	85.75400	123.748	135.000	138.317	65.492	14.569	271.346
B2S3	117.82000	-2.184	13.480	17.754	82.668	19.938	351.434
B3H7,C2v	39.48858	161.201	194.481	176.019	81.606	14.818	265.948
B3H7,Cs	39.48858	145.235	178.515	159.318	76.693	14.083	267.986
B3H9	41.50446	121.579	163.327	138.909	95.357	17.330	282.497
B3N3H6	80.50086	-528.221	-486.170	-512.000	93.888	16.221	287.642
B3O3CL3	186.78930	-1660.434	-1630.000	-1635.982	124.123	24.452	380.039
B3O3FCL2	170.33500	-1907.256	-1877.000	-1883.808	120.642	23.448	377.597
B3O3F2CL	153.88071	-2155.078	-2125.000	-2132.817	115.328	22.261	364.875
B3O3F3	137.42641	-2403.900	-2374.000	-2382.699	110.653	21.201	343.946
B4H4	47.27576	311.254	333.046	326.190	80.417	14.937	277.068
B4H10	53.32340	50.614	97.811	66.100	93.147	15.486	280.152
B4H12	55.33928	166.487	222.152	188.236	128.224	21.749	315.870
B5H9	63.12646	57.167	101.344	73.220	99.564	16.053	280.603
Ba	137.32700	178.803	185.710	185.000	20.786	6.197	170.247
Ba+	137.32645	687.852	688.562	694.050	20.786	6.197	176.010
BaBr	217.23100	-85.525	-66.358	-75.325	37.002	10.200	270.851
BaBr2	297.13500	-428.000	-396.574	-412.515	57.359	15.486	347.959
BaCL	172.77970	-146.168	-134.670	-136.291	36.440	9.877	258.839
BaCL+	172.77915	339.029	344.330	348.698	35.874	9.668	251.733
BaCL2	208.23240	-513.900	-497.812	-499.301	56.113	14.599	323.490
BaF	156.32540	-328.336	-317.016	-318.994	34.747	9.342	246.214
BaF+	156.32485	124.862	129.984	134.063	34.046	9.202	239.222
BaF2	175.32381	-825.441	-809.708	-812.003	53.272	13.437	298.673
BaH	138.33494	200.804	211.945	209.535	30.232	8.731	219.009
BaI	264.23147	-20.635	-7.130	-10.238	37.315	10.397	278.578
BaI2	391.13594	-304.230	-284.127	-288.440	57.632	15.790	361.977
BaO	153.32640	-126.963	-115.715	-117.948	32.898	9.014	235.460
BaO+	153.32585	502.235	507.285	511.705	37.467	9.470	244.661
BaOH	154.33434	-235.481	-220.000	-224.257	47.723	11.225	255.755
BaOH+	154.33379	190.716	200.000	202.019	48.054	11.303	251.098
Ba(OH)2	171.34168	-624.055	-600.000	-606.666	79.954	17.389	318.658
BaS	169.39300	29.315	40.634	38.871	35.532	9.556	248.864
Ba2	274.65400	344.605	358.419	355.964	37.016	11.359	290.710
Be	9.01218	317.803	319.745	324.000	20.786	6.197	136.276
Be+	9.01163	1223.504	1219.249	1229.701	20.786	6.197	142.039
Be++	9.01108	2986.804	2976.351	2993.002	20.786	6.197	136.275
BeBr	88.91618	123.475	137.677	132.446	32.598	8.971	229.591
BeBr2	168.82018	-246.900	-220.438	-234.062	53.252	12.838	273.241
BeCL	44.46488	47.832	54.365	56.693	31.650	8.861	218.100
BeCL2	79.91758	-373.620	-362.497	-361.539	51.048	12.081	250.263
BeF	28.01059	-179.336	-172.981	-170.625	29.872	8.711	205.754
BeF2	47.00899	-807.468	-796.701	-796.588	45.884	10.880	227.283
BeH	10.02012	333.604	339.780	342.252	29.224	8.648	176.823
BeH+	10.01957	1169.575	1169.554	1178.219	29.193	8.644	170.655
BeH2	11.02806	151.880	162.290	161.099	35.843	9.219	175.235
BeI	135.91665	198.365	206.905	207.454	33.401	9.089	237.579
BeI2	262.82112	-78.200	-63.062	-64.759	54.719	13.441	289.396
BeN	23.01892	418.275	424.552	427.000	30.089	8.725	208.770
BeO	25.01158	120.252	126.534	128.940	29.479	8.688	197.604

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^{\circ}(T)$ kJ/mol	T = 298.15 K: $C_p^{\circ}(T)$ J/K-mol	T = 298.15 K: $H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	T = 298.15 K: $S^{\circ}(T)$ J/K-mol
BeOH	26.01952	-110.516	-100.000	-99.718	43.642	10.798	217.058
BeOH+	26.01897	750.433	754.752	759.984	38.441	9.551	203.922
Be(OH)2	43.02686	-654.090	-635.000	-638.864	74.066	15.226	249.019
BeS	41.07818	238.315	244.669	247.095	30.786	8.780	210.286
Be2	18.02436	627.705	631.589	637.543	30.667	9.838	203.724
Be2CL4	159.83516	-842.246	-820.000	-819.605	105.515	22.641	366.340
Be2F4	94.01798	-1751.534	-1730.000	-1731.700	94.916	19.835	323.167
Be2O	34.02376	-48.224	-40.000	-37.034	47.783	11.190	227.956
Be2OF2	72.02057	-1221.159	-1204.110	-1204.574	76.152	16.585	298.919
Be2O2	50.02316	-422.564	-410.000	-411.635	46.287	10.929	243.042
Be3O3	75.03475	-1038.846	-1020.000	-1023.721	75.946	15.126	283.180
Be4O4	100.04633	-1665.128	-1640.000	-1649.295	88.657	15.834	296.472
Br	79.90400	105.673	117.933	111.870	20.786	6.197	175.019
Br+	79.90345	1251.730	1257.792	1257.927	20.787	6.197	176.874
Br-	79.90455	-225.198	-206.740	-219.000	20.786	6.197	163.493
BrCL	115.35670	5.382	22.233	14.789	35.011	9.407	240.049
BrF	98.90240	-67.873	-51.200	-58.851	32.959	9.021	228.988
BrF3	136.89921	-270.312	-244.814	-255.600	67.354	14.712	295.775
BrF5	174.89602	-447.975	-413.652	-428.800	101.335	19.175	323.253
BrO	95.90340	116.739	133.339	125.800	34.182	9.061	232.970
OBrO	111.90280	140.560	161.500	151.955	45.364	11.395	271.112
BrOO	111.90280	95.149	116.089	108.000	48.875	12.851	288.845
BrO3	127.90220	207.720	233.000	220.821	59.999	13.101	284.509
Br2	159.80800	21.185	45.705	30.910	36.057	9.725	245.469
BrBrO	175.80740	154.863	183.723	168.000	51.385	13.137	312.704
BrOBr	175.80740	95.240	124.100	107.639	50.168	12.399	290.823
C	12.01070	710.144	711.198	716.680	20.839	6.536	158.101
C+	12.01015	1802.795	1797.651	1809.444	20.974	6.649	154.663
C-	12.01125	582.095	589.346	588.314	20.787	6.219	159.003
CBr	91.91470	480.817	494.130	490.432	35.534	9.615	234.562
CBr2	171.81870	324.426	350.000	336.623	49.304	12.197	288.465
CBr3	251.72270	219.418	257.251	235.000	67.440	15.582	334.577
CBr4	331.62670	59.127	109.220	79.500	91.138	20.373	357.954
CCL	47.46340	423.216	428.860	432.611	32.268	9.395	224.556
CCLBr3	287.17540	45.432	87.856	65.000	89.299	19.568	357.617
CCL2	82.91610	211.517	221.752	222.940	46.305	11.423	264.872
CCL2Br2	242.72410	-8.692	26.063	10.000	87.053	18.692	348.490
CCL3	118.36880	56.728	71.553	71.128	63.500	14.400	303.100
CCL3Br	198.27280	-60.985	-33.899	-43.000	85.204	17.985	333.580
CCL4	153.82150	-112.759	-93.343	-95.600	82.890	17.159	309.467
CF	31.00910	233.235	238.701	242.300	30.056	9.065	213.034
CF+	31.00855	1136.867	1136.135	1145.564	29.642	8.697	201.509
CFBr3	270.72110	-138.243	-95.997	-120.000	84.257	18.243	345.725
CFCL	66.46180	14.943	25.000	25.846	42.962	10.902	259.150
CFCLBr2	226.26980	-192.498	-157.921	-175.000	82.338	17.498	343.087
CFCL2	101.91450	-118.217	-103.570	-105.000	59.121	13.217	298.917
CFCL2Br	181.81850	-251.731	-224.823	-235.000	80.108	16.731	330.773
CFCL3	137.36720	-299.764	-280.526	-283.700	78.071	16.064	309.785
CF2	50.00751	-196.951	-187.072	-186.600	38.915	10.351	240.831
CF2+	50.00696	938.999	942.680	949.341	38.541	10.342	246.731
CF2Br2	209.81551	-396.280	-361.881	-380.000	77.000	16.280	325.413
CF2CL	85.46021	-287.432	-272.963	-275.000	55.172	12.432	287.353
CF2CLBr	165.36421	-450.528	-423.799	-435.000	74.650	15.528	318.724
CF2CL2	120.91291	-505.681	-486.621	-490.800	72.477	14.881	300.908
CF3	69.00591	-478.891	-464.600	-467.400	49.642	11.491	264.521

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
CF3+	69.00536	412.076	420.170	423.617	49.339	11.541	254.540
CF3Br	148.90991	-663.244	-636.693	-648.800	69.270	14.444	297.695
CF3CL	104.45861	-717.991	-699.109	-704.200	66.887	13.791	285.424
CF4	88.00431	-945.850	-927.147	-933.120	61.052	12.730	261.459
CH	13.01864	588.745	594.033	597.371	29.175	8.625	183.040
CH+	13.01809	1621.943	1621.033	1630.571	29.154	8.628	171.673
CHBr3	252.73064	0.833	42.901	16.740	70.982	15.907	330.705
CHCL	48.47134	286.900	296.778	297.100	37.787	10.200	235.062
CHCLBr2	208.27934	-5.291	29.107	10.000	69.149	15.291	328.026
CHCL2	83.92404	83.000	97.469	95.800	53.900	12.800	285.500
CHCL2Br	163.82804	-59.730	-33.001	-45.000	67.395	14.730	316.478
CHCL3	119.37674	-117.005	-97.946	-102.700	66.879	14.305	296.374
CHF	32.01704	98.819	108.519	108.800	34.588	9.981	223.342
CHFBr2	191.82504	-189.360	-155.139	-175.000	64.915	14.360	316.925
CHFCL	67.46974	-94.291	-80.000	-83.145	45.077	11.146	268.507
CHFCLBr	147.37374	-243.787	-217.237	-230.000	62.869	13.787	310.691
CHFCL2	102.92244	-298.194	-279.313	-284.900	61.010	13.294	293.308
CHF2	51.01545	-249.820	-235.707	-238.900	43.062	10.920	258.000
CHF2Br	130.91945	-435.170	-408.797	-422.000	58.767	13.170	295.230
CHF3	70.01385	-704.867	-686.342	-693.300	51.082	11.567	259.689
CHI3	393.73205	193.717	218.799	210.874	75.072	17.157	355.622
CH2	14.02658	380.337	389.859	390.365	35.015	10.027	194.419
CH2Br2	173.83458	-27.384	6.657	-14.770	54.552	12.614	293.391
CH2CL	49.47958	108.220	122.332	119.200	43.173	10.980	242.634
CH2CLBr	129.38358	-57.191	-30.819	-45.000	52.726	12.191	287.290
CH2CL2	84.93258	-106.854	-88.151	-95.000	50.951	11.854	270.365
CH2F	33.02498	-42.929	-28.995	-31.800	42.442	11.129	233.700
CH2FBr	112.92898	-226.623	-200.428	-215.000	49.089	11.623	276.282
CH2FCL	68.47798	-276.952	-258.428	-265.700	47.046	11.252	264.426
CH2F2	52.02339	-462.993	-444.647	-452.300	42.880	10.693	246.711
CH2I2	267.83552	104.320	127.038	117.570	57.735	13.250	309.504
CH3	15.03452	136.292	150.047	146.658	38.417	10.366	194.009
CH3Br	94.93852	-48.353	-22.337	-37.740	42.455	10.613	245.959
CH3CL	50.48752	-92.286	-73.940	-81.870	40.741	10.416	234.396
CH3F	34.03292	-247.835	-229.667	-237.700	37.504	10.135	222.826
CH3I	141.93899	2.950	23.303	13.765	44.084	10.816	253.807
CH2OH	31.03392	-29.581	-11.485	-17.800	47.401	11.781	244.170
CH2OH+	31.03337	706.251	718.149	716.400	37.835	10.149	228.047
CH3O	31.03392	1.698	19.794	13.000	47.012	11.302	236.066
CH4	16.04246	-84.616	-66.626	-74.600	35.691	10.016	186.371
CH3OH	32.04186	-212.375	-190.046	-200.940	44.039	11.435	239.810
CH3OOH	48.04126	-152.919	-126.249	-139.000	61.690	13.919	276.504
CI	138.91517	560.707	568.358	570.201	36.908	9.494	241.318
CI2	265.81964	455.750	470.000	468.394	50.945	12.643	304.324
CI3	392.72411	389.152	410.000	405.984	70.550	16.831	361.033
CI4	519.62858	245.588	273.033	267.943	95.842	22.356	391.740
CN	26.01740	430.011	435.400	438.684	29.156	8.672	202.646
CN+	26.01685	1790.209	1789.400	1798.891	29.463	8.682	196.935
CN-	26.01795	55.214	66.800	63.885	29.151	8.671	196.576
CNN	40.02410	623.106	632.830	633.484	42.656	10.378	232.398
CO	28.01010	-119.206	-113.813	-110.535	29.141	8.671	197.660
CO+	28.00955	1239.118	1238.314	1247.789	29.137	8.671	203.230
COCL	63.46310	-27.551	-17.567	-16.000	45.073	11.551	265.195
COCL2	98.91610	-232.379	-217.804	-219.500	57.761	12.879	283.752

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
COFCL	82.46150	-441.397	-427.000	-429.493	52.397	11.904	276.705
COF2	66.00691	-651.134	-636.915	-640.000	47.365	11.134	258.971
COHCL	64.47104	-175.218	-161.000	-164.212	44.679	11.006	259.070
COHF	48.01644	-385.040	-371.000	-374.590	40.502	10.450	246.828
COS	60.07510	-151.642	-141.836	-141.700	41.549	9.942	231.650
CO2	44.00950	-402.875	-393.142	-393.510	37.135	9.365	213.787
CO2+	44.00895	934.122	937.658	944.688	41.799	10.566	228.017
COOH	45.01744	-223.813	-209.846	-213.000	43.610	10.813	251.736
CP	42.98446	511.447	517.860	520.162	29.910	8.715	216.257
CS	44.07570	269.842	275.307	278.550	29.799	8.708	210.558
CS2	76.14070	106.036	115.913	116.700	45.482	10.664	237.889
C2	24.02140	820.288	822.395	830.457	43.549	10.169	197.097
C2+	24.02085	1996.090	1992.000	2004.776	29.400	8.685	204.179
C2-	24.02195	472.091	480.395	480.767	29.241	8.676	196.599
C2CL	59.47440	523.302	530.000	534.083	45.046	10.781	241.948
C2CL2	94.92740	212.007	223.296	226.600	65.374	14.593	272.112
C2CL3	130.38040	174.121	190.000	190.272	76.033	16.150	328.166
C2CL4	165.83340	-43.806	-23.336	-24.200	94.920	19.606	341.034
C2CL6	236.73940	-175.329	-145.679	-148.200	136.348	27.129	398.632
C2F	43.01980	343.480	350.000	353.847	42.600	10.367	231.036
C2FCL	78.47280	19.890	31.000	33.766	62.627	13.877	266.386
C2FCL3	149.37880	-184.732	-164.441	-166.000	91.032	18.732	342.594
C2F2	62.01821	-157.932	-147.000	-144.666	60.114	13.266	249.570
C2F2CL2	132.92421	-355.773	-335.660	-337.837	89.506	17.936	326.491
C2F3	81.01661	-242.345	-227.000	-228.181	66.178	14.164	297.643
C2F3CL	116.46961	-532.328	-512.393	-515.200	83.917	17.128	322.389
C2F4	100.01501	-675.831	-656.073	-659.500	80.459	16.331	300.128
C2F6	138.01182	-1364.272	-1335.690	-1344.000	106.211	20.272	332.434
C2H	25.02934	555.752	562.093	566.200	42.000	10.449	213.304
C2HCL	60.48234	214.612	225.544	226.400	54.320	11.788	241.955
C2HCL3	131.38834	-34.105	-13.992	-17.500	80.016	16.605	324.942
C2HF	44.02774	30.246	41.000	41.692	52.268	11.446	231.573
C2HFCL2	114.93374	-184.907	-164.973	-168.648	77.324	16.259	320.191
C2HF2CL	98.47915	-348.917	-329.160	-333.654	76.650	15.263	304.242
C2HF3	82.02455	-505.328	-485.749	-491.000	69.191	14.328	292.665
C2H2,acetylene	26.03728	218.194	228.769	228.200	44.001	10.006	200.916
C2H2,vinylidene	26.03728	403.914	414.489	414.788	42.614	10.874	221.021
C2H2CL2	96.94328	-11.472	8.284	3.410	68.847	14.882	297.021
C2H2FCL	80.48868	-178.551	-158.973	-165.082	68.337	13.469	284.542
C2H2F2	64.03409	-348.880	-329.479	-336.400	60.237	12.480	266.054
CH2CO,ketene	42.03668	-61.372	-46.457	-49.576	51.740	11.796	251.442
O(CH)2O	58.03608	-225.682	-206.427	-212.000	60.409	13.682	272.483
HO(CO)2OH	90.03488	-749.122	-721.186	-731.800	86.178	17.322	320.649
C2H3,vinyl	27.04522	289.165	303.974	299.687	42.071	10.522	233.663
CH2Br-COOH	138.94802	-400.362	-364.613	-383.500	80.542	16.862	337.015
C2H3CL	62.49822	10.180	29.580	22.000	53.681	11.820	264.024
CH2CL-COOH	94.49672	-444.114	-416.034	-427.600	78.839	16.514	325.918
C2H3F	46.04362	-151.436	-132.214	-140.100	50.407	11.336	252.674
CH3CN	41.05192	54.336	73.481	66.430	52.246	12.094	243.460
CH3CO,acetyl	43.04462	-23.036	-3.887	-10.000	54.642	13.036	270.320
C2H4	28.05316	41.981	61.025	52.500	42.887	10.519	219.322
C2H4O,ethylen-o	44.05256	-63.465	-40.082	-52.635	47.624	10.831	242.870
CH3CHO,ethanal	44.05256	-179.087	-155.703	-166.190	55.319	12.897	263.952
CH3COOH	60.05196	-445.846	-418.123	-432.249	63.439	13.597	283.473
OHCH2COOH	76.05136	-600.007	-567.944	-583.000	87.076	17.007	318.614

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
C2H5	29.06110	106.473	129.750	118.658	50.484	12.185	247.118
C2H5Br	108.96510	-77.169	-41.632	-63.600	64.230	13.569	287.250
C2H6	30.06904	-95.743	-68.232	-83.852	52.501	11.892	229.221
CH3N2CH3	58.08244	132.174	168.356	148.699	78.063	16.525	289.823
C2H5OH	46.06844	-249.492	-217.641	-234.950	65.309	14.542	280.593
CH3OCH3	46.06844	-198.464	-166.613	-184.110	65.823	14.354	267.381
CH3O2CH3	62.06784	-142.653	-106.462	-125.500	80.719	17.153	308.414
CCN	38.02810	793.558	800.000	804.596	44.231	11.039	237.159
CNC	38.02810	673.558	680.000	684.915	45.042	11.357	233.804
OCCN	54.02754	196.406	207.188	210.000	56.145	13.594	278.187
C2N2	52.03480	296.385	307.162	309.100	57.085	12.715	242.204
C2O	40.02080	280.553	287.000	291.039	43.134	10.486	233.624
C2S2	88.15140	362.900	373.831	376.660	62.030	13.760	274.120
C3	36.03210	827.840	831.000	839.949	42.203	12.109	237.613
C3H3,1-propynl	39.05592	437.600	453.463	450.000	53.000	12.400	250.900
C3H3,2-propynl	39.05592	318.570	334.433	331.800	62.640	13.230	254.520
C3H4,allene	40.06386	178.315	198.412	190.920	58.880	12.605	243.630
C3H4,propyne	40.06386	171.869	191.966	184.900	60.731	13.031	248.428
C3H4,cyclo-	40.06386	265.726	285.823	277.100	52.883	11.374	243.605
C3H5,allyl	41.07180	150.856	175.186	163.594	63.387	12.739	258.886
C3H6,propylene	42.07974	6.449	35.014	20.000	64.433	13.551	266.668
C3H6,cyclo-	42.07974	41.890	70.455	53.300	55.572	11.410	237.488
C3H6O,propylox	58.07914	-108.125	-75.221	-93.720	72.370	14.405	281.523
C3H6O,acetone	58.07914	-233.343	-200.438	-217.150	74.207	16.193	295.660
C3H6O,propanal	58.07914	-203.327	-170.422	-186.000	84.472	17.327	300.873
C3H7,n-propyl	43.08768	85.640	118.439	100.500	71.211	14.860	289.586
C3H7,i-propyl	43.08768	78.493	111.292	93.300	66.314	14.807	289.494
C3H8	44.09562	-119.421	-82.388	-104.680	73.589	14.741	270.315
C3H8O,1propanol	60.09502	-272.719	-231.346	-255.200	84.978	17.519	323.367
C3H8O,2propanol	60.09502	-289.965	-248.592	-272.700	89.596	17.265	309.226
CNCOCN	80.04498	230.352	246.523	247.500	80.854	17.148	310.032
C3OS	84.09650	141.610	153.523	157.330	72.150	15.720	289.180
C3O2	68.03090	-108.723	-96.882	-93.638	67.370	15.085	276.816
C3S2	100.16210	396.510	408.494	412.500	74.780	15.990	288.340
C4	48.04280	1020.786	1025.000	1033.904	57.272	13.118	252.861
C4H2,butadiyne	50.05868	435.606	448.288	450.000	73.675	14.394	250.251
C4H4,1,3-cyclo-	52.07456	372.896	394.047	385.000	60.969	12.104	251.442
C4H6,butadiene	54.09044	94.870	124.488	110.000	79.810	15.130	278.780
C4H6,1butyne	54.09044	149.180	178.798	165.200	81.820	16.020	291.210
C4H6,2butyne	54.09044	129.060	158.678	145.700	78.020	16.640	284.210
C4H6,cyclo-	54.09044	144.142	173.761	156.700	64.414	12.558	262.076
C4H8,1-butene	56.10632	-17.660	20.426	-0.540	85.560	17.120	307.860
C4H8,cis2-buten	56.10632	-24.200	13.886	-7.400	80.150	16.800	301.310
C4H8,tr2-butene	56.10632	-28.510	9.576	-11.000	87.670	17.510	296.330
C4H8,isobutene	56.10632	-34.110	3.976	-17.100	88.090	17.010	293.200
C4H8,cyclo-	56.10632	14.866	52.952	28.400	70.565	13.534	264.509
(CH3COOH)2	120.10392	-957.069	-901.622	-929.015	137.254	28.053	414.396
C4H9,n-butyl	57.11426	46.733	89.053	66.530	97.670	19.797	328.519
C4H9,i-butyl	57.11426	39.003	81.323	57.320	95.530	18.317	318.649
C4H9,s-butyl	57.11426	53.462	95.783	71.000	87.392	17.538	334.126
C4H9,t-butyl	57.11426	34.690	77.011	51.700	78.225	17.010	319.719
C4H10,n-butane	58.12220	-145.019	-98.464	-125.790	98.657	19.229	309.881
C4H10,isobutane	58.12220	-152.927	-106.372	-134.990	96.643	17.936	295.493
C4N2	76.05620	511.401	524.285	529.200	86.326	17.799	290.524
C5	60.05350	1034.733	1040.000	1050.924	75.507	16.192	271.677

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
C5H6,1,3cyclo-	66.10114	120.764	151.436	134.300	75.369	13.536	274.154
C5H8,cyclo-	68.11702	19.043	58.183	33.900	81.276	14.857	291.380
C5H10,1-pentene	70.13290	-42.960	4.648	-21.280	108.200	21.680	347.110
C5H10,cyclo-	70.13290	-92.123	-44.515	-77.100	82.761	15.023	293.009
C5H11,pentyl	71.14084	21.388	73.230	45.810	119.150	24.422	368.649
C5H11,t-pentyl	71.14084	12.956	64.798	32.600	98.856	19.644	366.476
C5H12,n-pentane	72.14878	-170.944	-114.868	-146.760	120.040	24.184	349.560
C5H12,i-pentane	72.14878	-175.708	-119.632	-153.700	118.870	22.008	343.740
CH3C(CH3)2CH3	72.14878	-191.099	-135.023	-167.920	120.830	23.179	306.000
C6D5,phenyl	82.13471	299.821	327.565	315.740	94.997	15.919	300.504
C6D6	84.14881	41.833	73.861	58.157	100.398	16.325	282.629
C6H2	74.08008	650.392	665.181	670.000	103.919	19.608	298.911
C6H5,phenyl	77.10390	323.045	350.537	337.200	80.583	14.155	288.868
C6H5O,phenoxy	93.10330	31.492	63.323	47.700	94.143	16.208	307.896
C6H6	78.11184	68.684	100.410	82.880	81.935	14.196	269.159
C6H5OH,phenol	94.11124	-113.896	-77.830	-96.399	103.339	17.497	315.240
C6H10,cyclo-	82.14360	-21.871	26.791	-4.600	101.464	17.271	310.633
C6H12,1-hexene	84.15948	-68.190	-11.060	-41.950	130.800	26.240	386.350
C6H12,cyclo-	84.15948	-140.845	-83.715	-123.300	105.344	17.545	297.391
C6H13,n-hexyl	85.16742	-3.883	57.481	25.100	141.790	28.983	408.339
C6H14,n-hexane	86.17536	-195.622	-130.024	-166.920	142.590	28.702	388.850
C7H7,benzyl	91.13048	191.945	228.958	210.500	109.126	18.555	321.133
C7H8	92.13842	32.230	73.477	50.170	103.280	17.940	320.188
C7H8O,cresol-mx	108.13782	-154.136	-108.549	-132.298	128.027	21.838	360.118
C7H14,1-heptene	98.18606	-93.550	-26.899	-62.760	153.500	30.790	425.600
C7H15,n-heptyl	99.19400	-29.153	41.732	4.390	164.430	33.543	448.029
C7H16,n-heptane	100.20194	-221.001	-145.882	-187.780	165.180	33.221	428.089
C7H16,2-methylh	100.20194	-225.520	-150.401	-194.600	164.500	30.920	420.500
C8H8,styrene	104.14912	127.360	169.660	148.300	120.190	20.940	344.770
C8H10,ethylbenz	106.16500	7.640	58.409	29.920	127.400	22.280	360.630
C8H16,1-octene	112.21264	-118.940	-42.767	-83.590	176.100	35.350	464.840
C8H17,n-octyl	113.22058	-54.423	25.984	-16.320	187.070	38.103	487.729
C8H18,n-octane	114.22852	-246.530	-161.889	-208.750	187.780	37.780	467.350
C8H18,isooctane	114.22852	-256.180	-171.539	-224.010	188.410	32.170	423.090
C9H19,n-nonyl	127.24716	-79.694	10.234	-37.030	209.710	42.664	527.419
C10H8,naphthale	128.17052	129.867	174.274	150.580	131.920	20.713	333.267
C10H21,n-decyl	141.27374	-104.964	-5.514	-57.740	232.350	47.224	567.109
C12H9,o-bipheny	153.19986	401.141	451.889	427.730	163.049	26.589	405.113
C12H10,biphenyl	154.20780	155.346	210.329	182.130	166.179	26.784	388.944
Ca	40.07800	171.603	177.386	177.800	20.786	6.197	154.887
Ca+	40.07745	767.630	767.216	773.828	20.786	6.197	160.650
CaBr	119.98200	-34.725	-16.682	-24.869	36.390	9.856	253.125
CaBr2	199.88600	-402.800	-372.498	-387.197	60.287	15.603	310.134
CaCL	75.53100	-113.368	-102.995	-103.773	35.686	9.595	241.635
CaCL+	75.53045	457.829	462.005	467.191	34.811	9.361	233.154
CaCL2	110.98400	-500.101	-485.136	-485.243	59.050	14.857	286.396
CaF	59.07640	-285.536	-275.340	-276.404	33.671	9.132	229.138
CaF+	59.07585	251.661	255.660	260.665	32.824	9.003	222.299
CaF2	78.07481	-803.640	-789.032	-790.828	51.208	12.812	274.396
CaH	41.08594	220.704	230.721	229.409	29.896	8.705	201.844
CaI	166.98247	2.165	14.546	12.183	36.708	10.018	261.058
CaI2	293.88694	-275.370	-256.392	-259.320	60.835	16.051	326.578
CaO	56.07740	29.052	39.175	38.005	32.454	8.953	219.719
CaO+	56.07685	701.074	705.000	710.238	34.537	9.163	233.606
CaOH	57.08534	-184.357	-170.000	-173.307	46.733	11.050	238.853

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
CaOH+	57.08479	361.840	370.000	372.938	47.039	11.098	233.924
Ca(OH)2	74.09268	-614.931	-592.000	-598.339	77.001	16.592	292.045
CaS	72.14300	112.115	122.310	121.475	34.813	9.360	232.617
Ca2	80.15600	330.492	342.058	341.765	36.995	11.273	257.567
Cd	112.41100	105.603	111.850	111.800	20.786	6.197	167.750
Cd+	112.41045	979.557	979.606	985.754	20.786	6.197	173.513
CL	35.45300	115.029	119.620	121.301	21.838	6.272	165.192
CL+	35.45245	1372.413	1370.806	1378.800	22.959	6.386	167.558
CL-	35.45355	-240.155	-229.367	-233.958	20.786	6.197	153.358
CLCN	61.47040	123.531	133.510	134.200	44.960	10.669	236.144
CLF	54.45140	-64.609	-55.606	-55.701	32.085	8.908	217.943
CLF3	92.44821	-178.328	-160.500	-164.600	64.061	13.728	282.152
CLF5	130.44502	-255.930	-229.277	-238.000	97.167	17.930	310.257
CLO	51.45240	92.099	101.030	101.621	34.471	9.522	225.104
CLO2	67.45180	94.199	107.470	105.000	42.004	10.801	256.885
CL2	70.90600	-9.181	-9.181	0.000	33.949	9.181	223.082
CL2O	86.90540	67.305	80.826	79.000	47.811	11.695	267.951
Co	58.93320	422.082	426.853	428.442	23.024	6.360	179.520
Co+	58.93265	1186.712	1185.285	1193.003	22.271	6.292	178.348
Co-	58.93375	352.108	363.076	358.414	22.439	6.307	178.414
Cr	51.99610	391.283	395.340	397.480	20.786	6.197	174.313
Cr+	51.99555	1050.349	1048.209	1056.547	20.786	6.197	173.032
Cr-	51.99665	320.826	331.080	327.023	20.786	6.197	173.032
CrN	66.00280	496.231	504.623	505.009	30.754	8.778	230.556
CrO	67.99550	176.732	185.129	186.581	32.636	9.849	238.593
CrO2	83.99490	-118.737	-106.000	-108.043	41.971	10.694	265.575
CrO3	99.99430	-335.077	-318.000	-322.037	58.658	13.040	269.408
CrO3-	99.99485	-646.275	-623.000	-632.851	60.322	13.424	277.590
Cs	132.90545	70.303	78.014	76.500	20.786	6.197	175.602
Cs+	132.90490	452.204	453.718	458.402	20.786	6.197	169.838
Cs-	132.90600	18.600	32.508	24.797	20.786	6.197	169.839
CsBO2	175.71525	-701.368	-683.763	-686.902	59.435	14.466	315.586
CsBr	212.80945	-217.235	-197.264	-206.829	37.313	10.406	267.534
CsCL	168.35845	-252.360	-240.058	-242.229	36.957	10.131	256.082
CsF	151.90385	-373.860	-361.736	-364.215	35.878	9.645	243.249
CsH	133.91339	107.104	119.049	115.950	31.564	8.846	215.183
CsI	259.80992	-162.870	-148.561	-152.320	37.451	10.550	275.287
CsLi	139.84645	151.805	164.148	162.146	37.389	10.341	247.950
CsNO2	178.91095	-226.320	-205.594	-210.340	61.727	15.980	327.723
CsNO3	194.91035	-335.050	-309.984	-318.486	69.114	16.564	336.035
CsNa	155.89522	115.205	129.376	125.907	37.824	10.702	263.062
CsO	148.90485	27.752	39.803	37.587	39.188	9.835	248.512
CsOH	149.91279	-267.835	-251.550	-256.000	49.724	11.835	254.840
CsRb	218.37325	100.505	115.705	111.477	38.072	10.972	283.888
Cs2	265.81090	98.375	113.797	109.404	38.255	11.029	284.682
Cs2Br2	425.61890	-587.942	-548.000	-565.829	82.438	22.113	413.799
Cs2CO3	325.81980	-827.627	-798.131	-806.448	92.044	21.179	388.527
Cs2CL2	336.71690	-665.603	-641.000	-644.658	81.623	20.945	384.584
Cs2F2	303.80771	-911.247	-887.000	-891.859	79.717	19.389	358.063
Cs2I2	519.61984	-476.618	-448.000	-454.033	82.678	22.585	431.190
Cs2O	281.81030	-156.945	-137.183	-142.855	54.545	14.090	324.133
Cs2O+	281.80975	269.252	282.817	283.700	55.396	14.448	332.946
Cs2O2	297.80970	-264.496	-240.393	-247.069	73.070	17.426	340.960
Cs2O2H2	299.82558	-676.937	-644.367	-653.000	108.293	23.937	381.267
Cs2SO4	361.87350	-1141.640	-1104.446	-1117.652	110.165	23.988	411.179

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
Cu	63.54600	331.203	336.207	337.400	20.786	6.197	166.399
Cu+	63.54545	1082.882	1081.689	1089.080	20.786	6.197	160.636
Cu-	63.54655	206.521	217.723	212.719	20.786	6.197	160.636
CuCL	98.99900	81.619	91.213	91.090	35.262	9.471	237.210
CuF	82.54440	-21.633	-12.217	-12.550	33.380	9.083	226.498
CuF2	101.54281	-278.996	-265.167	-266.940	47.988	12.056	267.090
CuO	79.54540	296.519	305.863	306.270	35.693	9.751	234.621
Cu2	127.09200	475.410	485.418	485.340	36.585	9.930	241.724
Cu3CL3	296.99700	-287.294	-258.510	-258.570	124.572	28.724	429.533
D	2.01410	215.523	219.807	221.720	20.786	6.197	123.352
D+	2.01355	1534.127	1532.214	1540.324	20.786	6.197	117.585
D-	2.01465	136.555	147.037	142.753	20.786	6.197	117.592
DBr	81.91810	-45.705	-29.160	-37.036	29.228	8.668	204.484
DCL	37.46710	-102.208	-93.333	-93.547	29.170	8.661	192.773
DF	21.01251	-284.866	-276.169	-276.228	29.137	8.638	179.705
DOCL	53.46650	-89.864	-76.648	-79.539	38.585	10.325	240.321
DO2	34.01290	-3.578	9.387	6.487	35.845	10.065	232.883
DO2-	34.01345	-114.875	-95.713	-104.796	36.041	10.080	227.860
D2	4.02820	-8.569	-8.569	0.000	29.195	8.569	144.960
D2+	4.02766	1489.917	1492.289	1498.568	29.510	8.651	156.735
D2-	4.02875	226.447	241.213	235.161	30.315	8.714	158.261
D2O	20.02760	-259.170	-246.261	-249.210	34.265	9.960	198.341
D2O2	36.02700	-155.866	-138.616	-144.300	45.242	11.566	242.098
D2S	36.09320	-34.095	-21.114	-24.007	35.795	10.089	215.316
F	18.99840	72.862	77.274	79.380	22.747	6.518	158.752
F+	18.99785	1760.106	1758.321	1766.816	23.497	6.711	161.730
F-	18.99895	-261.289	-250.680	-255.092	20.786	6.197	145.578
FCN	45.01580	24.199	34.000	34.328	41.757	10.129	224.607
FCO	47.00850	-189.806	-180.000	-179.418	38.880	10.388	248.992
FO	34.99780	99.624	108.377	109.012	31.995	9.388	216.396
FO2,FOO	50.99720	14.144	27.237	25.400	44.453	11.256	259.510
FO2,OFO	50.99720	368.062	381.154	378.600	41.126	10.538	251.289
F2	37.99681	-8.825	-8.825	0.000	31.304	8.825	202.792
F2O	53.99621	13.588	26.754	24.500	43.495	10.912	247.508
F2O2	69.99561	5.422	22.927	19.200	62.073	13.778	277.214
FS2F	102.12681	-351.030	-333.381	-336.435	66.042	14.595	294.087
Fe	55.84500	408.621	413.128	415.471	25.675	6.850	180.490
Fe+	55.84445	1177.282	1175.592	1184.218	26.068	6.936	181.858
Fe-	55.84555	386.696	397.401	393.338	25.023	6.642	180.200
Fe(CO)5	195.89550	-760.995	-729.521	-727.850	170.705	33.145	439.291
FeCL	91.29800	240.663	249.760	251.040	38.223	10.377	257.576
FeCL2	126.75100	-155.278	-141.590	-141.001	57.571	14.277	299.287
FeCL3	162.20400	-1077.318	-1059.040	-1059.104	77.703	18.214	344.211
FeO	71.84440	242.203	251.050	251.040	31.406	8.837	241.926
Fe(OH)2	89.85968	-344.745	-323.090	-330.536	71.505	14.209	283.092
Fe2CL4	253.50200	-461.220	-433.843	-431.370	125.876	29.849	464.506
Fe2CL6	324.40800	-694.825	-658.268	-654.378	173.665	40.448	536.945
Ga	69.72300	265.449	271.089	272.000	25.347	6.551	169.045
Ga+	69.72245	850.491	849.934	856.688	20.786	6.197	161.793
GaBr	149.62700	-27.900	-10.000	-17.968	36.557	9.932	251.830
GaBr2	229.53100	-163.206	-133.046	-149.181	55.076	14.025	323.444
GaBr3	309.43500	-312.000	-269.580	-292.963	78.467	19.037	359.416
GaCL	105.17600	-79.231	-69.000	-69.621	35.727	9.609	240.254
GaCL2	140.62900	-234.492	-219.671	-220.979	53.855	13.513	302.930
GaCL3	176.08200	-450.000	-430.588	-432.625	74.777	17.375	324.528

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
GaF	88.72140	-241.690	-231.637	-232.608	33.363	9.081	227.816
GaF2	107.71981	-528.828	-514.363	-516.712	47.811	12.116	278.721
GaF3	126.71821	-936.700	-917.822	-921.477	66.213	15.223	292.183
GaH	70.73094	205.650	215.524	214.323	29.439	8.673	199.779
GaI	196.62747	34.762	47.000	44.871	36.870	10.109	259.781
GaI2	323.53194	-43.426	-24.590	-28.955	55.962	14.471	338.523
GaI3	450.43641	-136.000	-110.566	-115.877	80.205	20.123	384.816
GaO	85.72240	137.899	147.879	146.824	32.226	8.925	230.825
GaOH	86.73034	-154.214	-140.000	-143.630	45.169	10.584	235.153
Ga2Br2	299.25400	-157.757	-121.957	-136.964	81.379	20.793	379.766
Ga2Br4	459.06200	-446.412	-386.092	-415.820	127.693	30.592	471.809
Ga2Br6	618.87000	-714.840	-630.000	-673.689	174.122	41.151	568.127
Ga2CL2	210.35200	-240.461	-220.000	-220.973	79.726	19.488	353.537
Ga2CL4	281.25800	-629.642	-600.000	-602.327	122.739	27.315	419.676
Ga2CL6	352.16400	-998.823	-960.000	-962.464	165.885	36.360	492.759
Ga2F2	177.44281	-623.379	-603.274	-606.231	75.221	17.148	320.316
Ga2F4	215.43961	-1347.656	-1318.726	-1325.003	110.133	22.653	369.066
Ga2F6	253.43642	-2047.755	-2010.000	-2017.624	146.582	30.131	426.411
Ga2I2	393.25494	-7.977	16.499	13.521	82.003	21.498	399.064
Ga2I4	647.06388	-191.852	-154.180	-159.268	130.064	32.584	509.437
Ga2I6	900.87282	-360.868	-310.000	-317.295	177.309	43.573	616.298
Ga2O	155.44540	-111.620	-96.000	-99.457	48.462	12.163	284.141
Ge	72.64000	360.401	365.038	367.800	30.733	7.399	167.914
Ge+	72.63945	1128.779	1127.218	1134.984	21.025	6.206	168.098
Ge-	72.64055	238.422	249.255	245.403	21.985	6.981	180.836
GeBr	152.54400	127.574	144.470	137.438	37.250	9.864	257.228
GeBr2	232.44800	-75.156	-46.000	-60.963	55.757	14.193	319.173
GeBr3	312.35200	-137.581	-96.164	-119.031	78.139	18.549	363.176
GeBr4	392.25600	-314.963	-261.287	-291.000	101.687	23.963	396.196
GeCL	108.09300	59.431	68.658	69.030	36.990	9.599	245.907
GeCL2	143.54600	-184.277	-170.459	-171.000	53.785	13.277	295.835
GeCL3	178.99900	-284.510	-266.102	-266.951	76.258	17.559	335.213
GeCL4	214.45200	-521.137	-498.138	-500.000	95.919	21.137	348.403
GeF	91.63840	-79.737	-70.688	-70.593	34.784	9.144	234.014
GeF2	110.63681	-585.787	-572.326	-574.000	47.848	11.787	270.791
GeF3	129.63521	-821.011	-803.137	-806.333	66.181	14.678	297.728
GeF4	148.63361	-1207.443	-1185.156	-1190.150	81.603	17.293	301.936
GeH4	76.67176	(a)	(a)	90.793	45.017	(a)	217.264
GeI	199.54447	200.964	212.198	210.969	37.083	10.005	264.745
GeO	88.63940	-46.476	-37.500	-37.694	30.804	8.782	223.894
GeO2	104.63880	-117.430	-104.114	-106.172	47.061	11.258	241.255
GeS	104.70500	83.384	92.432	92.525	33.710	9.141	235.582
GeS2	136.77000	105.750	119.210	118.818	54.755	13.068	266.900
Ge2	145.28000	460.803	470.076	471.499	41.681	10.696	256.458
H	1.00794	211.801	216.035	217.999	20.786	6.197	114.718
H+	1.00739	1530.049	1528.085	1536.246	20.786	6.197	108.948
H-	1.00849	132.834	143.265	139.031	20.786	6.197	108.961
HALO	43.98888	-8.114	5.000	1.821	40.996	9.935	219.696
HALO2	59.98828	-367.454	-350.000	-355.474	51.256	11.981	254.826
HBO	27.81834	-219.788	-210.000	-210.621	35.307	9.167	202.696
HBO+	27.81779	1166.125	1169.716	1175.220	34.745	9.095	214.568
HBO2	43.81774	-571.128	-557.000	-560.210	44.295	10.918	240.817
HBS	43.88394	40.922	50.782	50.208	36.740	9.286	214.955
HBS+	43.88339	1119.323	1122.986	1129.459	41.255	10.136	226.304
HBr	80.91194	-44.938	-28.444	-36.290	29.141	8.648	198.700

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
HCN	27.02534	123.847	133.470	133.082	35.857	9.235	201.824
HCO	29.01804	32.408	42.036	42.398	34.591	9.989	224.336
HCO+	29.01749	823.988	827.418	833.034	34.172	9.046	201.764
HCCN	39.03604	598.565	609.241	610.431	54.238	11.866	240.596
HCCO	41.02874	164.903	175.584	176.568	49.975	11.665	246.408
HCL	36.46094	-100.950	-92.125	-92.310	29.136	8.640	186.903
HD	3.02204	-8.186	0.333	0.323	29.200	8.509	143.801
HD+	3.02149	1488.179	1490.500	1496.793	29.334	8.614	155.552
HDO	19.02144	-255.206	-242.348	-245.280	33.798	9.926	199.517
HDO2	35.02084	-151.577	-134.378	-140.242	43.779	11.335	243.581
HF	20.00634	-281.899	-273.252	-273.300	29.137	8.599	173.777
HI	127.91241	17.703	28.535	26.359	29.157	8.656	206.592
HNC	27.02534	184.377	194.000	194.378	40.271	10.001	205.511
HNCO	43.02474	-129.023	-115.060	-118.057	45.078	10.966	238.265
HNO	31.01404	92.091	105.000	102.033	33.880	9.942	220.920
HNO2	47.01344	-90.049	-72.800	-78.452	46.320	11.597	254.071
HNO3	63.01284	-145.789	-124.200	-133.913	54.109	11.876	266.878
HOCL	52.46034	-85.965	-72.800	-75.740	37.293	10.225	236.567
HOF	36.00574	-106.987	-94.000	-96.898	35.940	10.088	226.757
HO2	33.00674	2.018	14.932	12.020	34.893	10.002	229.106
HO2-	33.00729	-108.1684	-89.057	-97.923	37.720	10.245	226.610
HPO	47.98110	-66.934	-53.000	-56.869	35.829	10.065	235.683
HSO3F	100.06954	-768.134	-742.055	-753.120	75.245	15.014	297.272
H2	2.01588	-8.468	-8.468	0.000	28.836	8.468	130.681
H2+	2.01533	1486.089	1488.360	1494.672	29.289	8.583	142.370
H2-	2.01643	226.548	241.213	235.168	29.556	8.621	143.747
HBOH	28.82628	-59.665	-45.643	-48.724	43.082	10.941	234.021
HCHO,formaldehy	30.02598	-118.600	-104.738	-108.580	35.388	10.020	218.764
HCOOH	46.02538	-389.498	-371.296	-378.570	45.680	10.928	248.990
H2F2	40.01269	-583.793	-566.500	-569.924	58.132	13.869	260.905
H2O	18.01528	-251.730	-238.922	-241.826	33.588	9.904	188.829
H2O+	18.01473	971.667	978.278	981.602	33.683	9.934	195.378
H2O2	34.01468	-147.039	-129.891	-135.880	42.388	11.159	234.527
H2S	34.08088	-30.558	-17.678	-20.600	34.255	9.958	205.816
H2SO4	98.07848	-749.240	-719.000	-732.732	84.401	16.509	299.289
H2BOH	29.83422	-300.256	-282.000	-289.634	42.642	10.622	230.910
HB(OH)2	45.83362	-656.596	-634.000	-644.439	57.145	12.158	257.009
H3BO3	61.83302	-1017.920	-990.984	-1004.360	70.040	13.560	268.230
H3B3O3	83.45502	-1219.364	-1190.000	-1203.761	80.615	15.603	286.152
H3B3O6	131.45322	-2287.384	-2245.000	-2263.688	133.912	23.697	359.908
H3F3	60.01903	-898.940	-873.000	-883.677	73.884	15.263	280.947
H3O+	19.02267	587.954	598.798	598.000	35.485	10.046	193.139
(HCOOH)2	92.05076	-840.575	-804.171	-820.943	96.142	19.632	332.785
H4F4	80.02537	-1208.586	-1174.000	-1186.932	104.022	21.654	350.016
H5F5	100.03172	-1518.233	-1475.000	-1490.188	134.161	28.045	417.286
H6F6	120.03806	-1839.880	-1788.000	-1805.545	163.735	34.334	486.619
H7F7	140.04440	-2140.526	-2080.000	-2099.699	194.438	40.827	548.654
He	4.00260	-6.197	-6.197	0.000	20.786	6.197	126.154
He+	4.00205	2372.324	2372.324	2378.521	20.786	6.197	131.915
Hg	200.59000	55.183	64.526	61.380	20.786	6.197	174.972
Hg+	200.58945	1068.446	1071.591	1074.643	20.786	6.197	180.735
HgBr2	360.39800	-106.970	-73.107	-91.312	60.277	15.658	320.227
I	126.90447	100.563	107.161	106.760	20.786	6.197	180.789
I+	126.90392	1115.154	1115.554	1121.351	20.786	6.197	182.644
I-	126.90502	-200.793	-187.998	-194.596	20.786	6.197	169.262

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
IF5	221.89649	-861.044	-832.383	-841.000	102.750	20.044	334.712
IF7	259.89329	-985.623	-948.137	-961.500	135.652	24.123	353.126
I2	253.80894	52.304	65.500	62.420	36.887	10.116	260.687
In	114.81800	234.501	241.111	240.700	20.830	6.199	173.782
In+	114.81745	0.799	1.212	6.996	20.786	6.197	168.014
InBr	194.72200	-64.200	-45.330	-54.116	36.824	10.084	259.617
InBr2	274.62600	-164.153	-133.023	-149.729	55.831	14.424	333.556
InBr3	354.53000	-276.500	-233.110	-256.587	79.889	19.913	373.477
InCL	150.27100	-81.900	-70.699	-72.148	36.138	9.752	248.274
InCL2	185.72400	-215.440	-199.649	-201.483	54.844	13.956	314.208
InCL3	221.17700	-388.000	-367.618	-369.693	76.722	18.307	339.170
InF	133.81640	-202.637	-191.614	-193.420	34.149	9.217	236.248
InF2	152.81481	-469.776	-454.340	-457.187	49.435	12.589	290.910
InF3	171.81321	-879.400	-859.552	-863.080	69.566	16.320	308.291
InH	115.82594	206.333	217.177	215.017	29.583	8.684	207.665
InI	241.72247	16.146	29.354	26.417	37.101	10.271	267.446
InI2	368.62694	-54.373	-34.567	-39.461	56.620	14.913	349.839
InI3	495.53141	-126.288	-99.884	-105.436	81.093	20.852	398.640
InO	130.81740	136.951	147.901	145.993	33.548	9.042	238.914
InOH	131.82534	-135.184	-120.000	-124.447	46.021	10.737	243.709
In2Br2	389.44400	-217.740	-180.000	-196.305	81.936	21.435	398.293
In2Br4	549.25200	-468.307	-406.047	-436.509	128.879	31.798	496.377
In2Br6	709.06000	-671.780	-585.000	-628.683	176.457	43.097	603.457
In2CL2	300.54200	-252.401	-230.000	-232.177	80.698	20.224	372.424
In2CL4	371.44800	-608.582	-577.000	-579.126	125.237	29.457	455.968
In2CL6	442.35400	-920.763	-880.000	-882.340	169.253	38.423	527.664
In2F2	267.63281	-550.274	-528.229	-532.234	77.254	18.040	339.263
In2F4	305.62961	-1309.551	-1278.681	-1284.788	114.222	24.763	400.833
In2F6	343.62642	-1993.567	-1953.872	-1960.000	155.898	33.567	468.351
In2I2	483.44494	-49.872	-23.456	-27.814	82.382	22.058	416.357
In2I4	737.25388	-232.612	-193.000	-199.143	130.687	33.469	529.944
In2I6	991.06282	-364.808	-312.000	-319.720	178.886	45.088	644.765
In2O	245.63540	-47.560	-30.000	-34.764	50.591	12.797	301.927
K	39.09830	82.803	89.891	89.000	20.786	6.197	160.342
K+	39.09775	507.810	508.701	514.008	20.786	6.197	154.578
K-	39.09885	28.221	41.506	34.418	20.786	6.197	154.579
KALF4	142.07345	-1929.278	-1900.000	-1907.857	104.398	21.421	351.969
KBO2	81.90810	-682.114	-665.132	-668.023	58.945	14.091	296.738
KBr	119.00230	-189.360	-170.012	-179.251	36.928	10.109	250.537
KCN	65.11570	67.040	79.516	79.496	50.858	12.456	253.150
KCL	74.55130	-224.460	-212.781	-214.575	36.505	9.885	239.094
KF	58.09670	-337.900	-326.399	-328.445	35.233	9.455	226.630
KH	40.10624	116.604	127.926	125.399	31.049	8.795	198.030
KI	166.00277	-138.700	-125.014	-128.456	37.129	10.244	258.291
KLi	46.03930	160.505	172.225	170.702	37.170	10.197	230.171
KNO2	85.10380	-207.840	-187.737	-192.497	61.132	15.343	302.355
KNO3	101.10320	-331.750	-307.307	-315.833	68.530	15.917	311.473
KNa	62.08807	121.830	135.378	132.404	37.783	10.574	245.845
KO	55.09770	55.252	66.680	64.733	35.352	9.481	241.198
KOH	56.10564	-243.675	-228.013	-232.000	49.185	11.675	238.287
K2	78.19660	115.805	129.981	126.546	37.982	10.741	249.760
K2+	78.19605	513.800	521.778	524.661	38.133	10.861	259.959
K2Br2	238.00460	-559.696	-521.000	-538.744	81.657	20.952	376.376
K2CO3	138.20550	-831.165	-802.915	-811.649	89.939	19.516	345.508
K2C2N2	130.23140	-33.154	-8.201	-8.368	110.264	24.786	373.135

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	T = 298.15 K: $C_p^o(T)$ J/K-mol	T = 298.15 K: $H^o(T) - H^o(0)$ kJ/mol	T = 298.15 K: $S^o(T)$ J/K-mol
K2CL2	149.10260	-635.357	-612.000	-615.394	80.699	19.963	350.390
K2F2	116.19341	-878.001	-855.000	-859.875	77.835	18.126	321.150
K2I2	332.00554	-440.372	-413.000	-418.915	82.040	21.457	393.955
K2O	94.19600	-87.945	-69.429	-74.087	54.180	13.858	286.548
K2O+	94.19545	354.252	366.571	368.390	54.874	14.138	297.123
K2O2	110.19540	-207.856	-185.000	-191.566	70.589	16.290	306.461
K2O2H2	112.21128	-663.385	-632.061	-641.000	105.593	22.385	342.859
K2SO4	174.25920	-1118.135	-1082.187	-1095.851	108.055	22.284	364.963
Kr	83.80000	-6.197	-6.197	0.000	20.786	6.197	164.086
Kr+	83.79945	1350.756	1350.756	1356.954	20.786	6.197	175.613
Li	6.94100	153.103	157.735	159.300	20.786	6.197	138.783
Li+	6.94045	679.522	677.957	685.719	20.786	6.197	133.018
Li-	6.94155	87.277	98.107	93.475	20.786	6.197	133.020
LiALF4	109.91615	-1876.822	-1850.000	-1857.288	99.340	19.534	326.521
LiBO2	49.75080	-665.780	-651.254	-652.352	57.163	13.428	272.380
LiBr	86.84500	-160.336	-143.444	-151.163	33.932	9.173	224.337
LiCL	42.39400	-202.840	-193.617	-193.780	33.254	9.060	212.860
LiF	25.93940	-349.773	-340.728	-340.945	31.292	8.828	200.300
LiH	7.94894	130.578	139.444	139.264	29.731	8.686	170.907
LiI	133.84547	-94.560	-83.330	-85.270	34.551	9.290	232.220
LiN	20.94770	325.721	334.688	334.720	32.839	8.999	208.248
LiNO2	52.94650	-215.400	-197.753	-202.031	56.959	13.369	265.014
LiNO3	68.94590	-325.500	-303.513	-311.585	64.061	13.915	278.287
LiO	22.94040	63.552	72.524	72.914	32.317	9.362	211.123
LiOF	41.93880	-102.875	-89.491	-92.048	43.032	10.827	246.026
LiOH	23.94834	-240.337	-227.131	-229.000	46.026	11.337	214.377
LiON	36.94710	168.611	181.918	179.912	44.424	11.301	245.335
Li2	13.88200	206.225	215.489	215.900	36.103	9.675	197.000
Li2+	13.88145	711.622	714.689	721.611	36.978	9.989	207.572
Li2Br2	173.69000	-512.784	-479.000	-495.834	75.105	16.950	317.489
Li2CL2	84.78800	-613.445	-595.000	-597.539	72.625	15.906	292.645
Li2F2	51.87881	-949.089	-931.000	-935.323	64.770	13.766	261.916
Li2I2	267.69094	-380.460	-358.000	-362.801	76.762	17.659	334.607
Li2O	29.88140	-180.131	-166.527	-167.339	50.286	12.792	232.985
Li2O+	29.88085	426.066	433.473	439.095	51.385	13.029	242.552
Li2O2	45.88080	-292.946	-275.002	-279.398	59.412	13.548	258.643
Li2O2H2	47.89668	-752.579	-726.167	-737.000	79.887	15.579	270.726
Li2SO4	109.94460	-1061.469	-1030.432	-1041.816	101.805	19.653	322.826
Li3+	20.82245	743.301	751.000	756.591	54.285	13.289	245.270
Li3Br3	260.53500	-850.676	-800.000	-824.639	118.950	26.037	401.354
Li3CL3	127.18200	-1000.668	-973.000	-976.107	115.506	24.561	367.816
Li3F3	77.81821	-1545.134	-1518.000	-1524.597	102.920	20.537	316.818
Li3I3	401.53641	-639.690	-606.000	-612.457	121.601	27.233	425.290
Mg	24.30500	140.903	145.882	147.100	20.786	6.197	148.649
Mg+	24.30445	884.850	883.631	891.047	20.786	6.197	154.412
MgBr	104.20900	-3.425	13.814	6.163	35.664	9.588	244.976
MgBr2	184.11300	-321.500	-292.001	-306.743	58.550	14.757	296.432
MgCL	59.75800	-64.068	-54.498	-54.705	34.837	9.363	233.423
MgCL+	59.75745	636.824	640.196	646.339	35.447	9.516	228.559
MgCL2	95.21100	-413.070	-398.910	-399.170	56.548	13.901	272.242
MgF	43.30340	-241.236	-231.844	-232.267	32.580	8.969	221.097
MgF+	43.30285	507.898	511.093	516.868	32.606	8.969	215.334
MgF2	62.30181	-748.120	-734.316	-735.498	52.293	12.622	247.556
MgF2+	62.30126	570.277	577.884	582.692	52.450	12.415	258.148
MgH	25.31294	221.104	230.317	229.786	29.587	8.682	193.197

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
MgI	151.20947	51.465	63.042	61.206	36.078	9.741	252.815
MgI2	278.11394	-187.000	-168.825	-171.706	59.364	15.294	313.820
MgN	38.31170	279.707	289.021	288.696	32.733	8.989	224.838
MgO	40.30440	23.352	32.671	32.261	32.111	8.909	213.318
MgOH	41.31234	-143.553	-130.000	-132.429	46.497	11.124	232.622
MgOH+	41.31179	605.581	612.937	615.769	43.216	10.188	220.827
Mg(OH)2	58.31968	-569.127	-547.000	-551.996	80.668	17.132	271.597
MgS	56.37000	111.415	120.806	120.649	34.237	9.234	225.447
Mg2	48.61000	276.971	286.930	286.513	24.199	9.542	240.843
Mg2F4	124.60361	-1739.512	-1711.904	-1718.369	107.502	21.143	337.018
Mn	54.93805	276.203	281.197	282.400	20.786	6.197	173.718
Mn+	54.93750	999.674	998.470	1005.871	20.786	6.197	175.000
Mo	95.94000	652.303	656.888	658.500	20.786	6.197	181.953
Mo+	95.93945	1342.815	1341.203	1349.013	20.786	6.197	180.671
Mo-	95.94055	574.127	584.910	580.325	20.786	6.197	180.671
MoO	111.93940	347.752	356.677	358.005	35.432	10.253	244.759
MoO2	127.93880	-26.265	-13.000	-15.558	42.011	10.707	273.915
MoO3	143.93820	-377.605	-360.000	-364.412	59.516	13.193	276.516
MoO3-	143.93875	-668.803	-645.000	-655.243	60.762	13.560	284.670
Mo2O6	287.87640	-1175.210	-1140.000	-1149.447	130.228	25.763	387.433
Mo3O9	431.81460	-1942.815	-1890.000	-1902.031	205.375	40.784	508.711
Mo4O12	575.75280	-2680.421	-2610.000	-2625.527	280.018	54.894	609.496
Mo5O15	719.69100	-3398.026	-3310.000	-3329.108	353.826	68.917	709.311
N	14.00670	466.483	470.818	472.680	20.786	6.197	153.302
N+	14.00615	1875.011	1873.149	1882.128	21.285	7.117	159.799
N-	14.00725	467.039	477.572	473.538	21.009	6.498	159.930
NCO	42.01680	121.649	131.378	131.847	39.989	10.198	232.229
ND	16.02080	347.091	355.710	355.739	29.159	8.648	187.234
ND2	18.03490	174.874	187.778	184.837	34.415	9.962	204.335
ND3	20.04901	-64.986	-47.797	-54.752	38.225	10.234	203.931
NF	33.00510	224.252	233.000	232.990	30.228	8.738	213.020
NF2	52.00351	23.840	37.000	34.421	41.058	10.582	249.638
NF3	71.00191	-143.555	-125.982	-131.700	53.497	11.855	260.812
NH	15.01464	348.431	357.000	357.032	29.193	8.601	181.227
NH+	15.01409	1656.293	1658.664	1665.788	32.775	9.495	187.651
NHF	34.01304	101.970	114.952	112.000	35.234	10.030	230.806
NHF2	53.01145	-113.807	-96.413	-103.000	43.384	10.807	252.814
NH2	16.02258	179.197	192.000	189.135	33.857	9.938	194.996
NH2F	35.02098	-85.105	-67.889	-75.000	36.474	10.105	229.534
NH3	17.03052	-55.983	-38.946	-45.940	35.630	10.043	192.770
NH2OH	33.02992	-61.236	-39.859	-50.000	46.472	11.236	236.181
NH4+	18.03791	634.926	650.000	644.905	34.764	9.979	186.095
NO	30.00610	82.092	90.767	91.271	29.862	9.179	210.748
NO+	30.00555	982.140	984.617	990.810	29.123	8.670	198.234
NOCL	65.45910	41.334	54.600	52.699	44.623	11.364	261.590
NOF	49.00450	-75.720	-62.633	-65.000	41.530	10.720	248.224
NOF3	87.00131	-200.698	-178.785	-187.000	68.067	13.698	277.731
NO2	46.00550	23.985	37.000	34.193	37.177	10.208	240.171
NO2-	46.00605	-210.213	-191.000	-200.036	37.215	10.177	236.219
NO2CL	81.45850	0.295	17.901	12.500	53.245	12.205	272.128
NO2F	65.00390	-120.347	-102.919	-109.000	48.999	11.347	259.287
NO3	62.00490	60.169	77.524	71.128	46.935	10.959	252.623
NO3-	62.00545	-321.553	-298.000	-310.780	44.724	10.773	245.638
NO3F	81.00330	0.556	22.324	15.000	66.959	14.444	293.171
N2	28.01340	-8.670	-8.670	0.000	29.124	8.670	191.610

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
N2+	28.01285	1500.837	1503.310	1509.508	29.137	8.671	197.663
N2-	28.01395	139.509	154.377	148.183	29.194	8.674	204.539
NCN	40.02410	490.276	500.000	500.457	41.946	10.180	225.814
N2D2,cis	32.04160	192.549	209.788	202.857	39.025	10.308	224.095
N2F2	66.01021	49.505	67.000	62.374	56.569	12.869	268.216
N2F4	104.00701	-39.812	-13.491	-22.000	88.384	17.812	317.531
N2H2	30.02928	201.862	219.000	211.859	35.045	9.997	218.333
NH2NO2	62.02808	-38.164	-12.346	-26.000	56.372	12.164	268.548
N2H4	32.04516	83.731	109.337	95.180	48.430	11.449	238.466
N2O	44.01280	72.019	85.029	81.600	38.628	9.581	220.010
N2O+	44.01225	1322.333	1329.146	1332.957	42.263	10.623	233.859
N2O3	76.01160	69.510	91.200	86.631	72.733	17.121	314.736
N2O4	92.01100	-5.630	20.400	11.111	79.168	16.741	304.451
N2O5	108.01040	-7.497	22.873	13.300	95.332	20.797	355.717
N3	42.02010	426.429	439.434	436.000	36.175	9.571	223.071
N3H	43.02804	283.053	300.292	294.000	44.219	10.947	239.330
Na	22.98977	101.303	107.763	107.500	20.786	6.197	153.719
Na+	22.98922	603.346	603.608	609.543	20.786	6.197	147.955
Na-	22.99032	42.256	54.913	48.453	20.786	6.197	147.956
NaALF4	125.96492	-1878.650	-1850.000	-1857.842	103.092	20.809	341.700
NaBO2	65.79957	-647.132	-630.778	-633.449	58.139	13.683	286.323
NaBr	102.89377	-155.750	-137.030	-145.929	36.338	9.821	241.224
NaCN	49.00717	82.140	93.989	94.266	50.179	12.126	243.370
NaCL	58.44277	-191.160	-180.109	-181.545	35.798	9.615	229.797
NaF	41.98817	-304.382	-293.509	-295.157	34.221	9.225	217.613
NaH	23.99771	132.104	142.798	140.835	30.294	8.731	188.391
NaI	149.89424	-100.590	-87.532	-90.638	36.643	9.952	248.981
NaLi	29.93077	168.605	179.697	178.598	36.910	9.993	219.434
NaNO2	68.99527	-181.100	-161.625	-166.293	60.250	14.807	289.624
NaNO3	84.99467	-300.930	-277.115	-285.529	67.667	15.401	300.084
NaO	38.98917	96.752	107.552	106.505	35.084	9.753	228.583
NaOH	39.99711	-202.398	-187.364	-191.000	47.967	11.398	228.978
NaOH+	39.99656	672.168	681.004	683.862	49.257	11.695	242.630
Na2	45.97954	131.936	144.856	142.339	37.574	10.403	230.246
Na2Br2	205.78754	-500.440	-463.000	-480.848	80.319	19.592	351.048
Na2CL2	116.88554	-583.101	-561.000	-564.402	79.035	18.699	327.529
Na2F2	83.97635	-850.745	-829.000	-834.063	74.929	16.682	297.907
Na2I2	299.78848	-377.116	-351.000	-356.870	81.056	20.246	368.732
Na2O	61.97894	-30.970	-13.710	-16.560	56.773	14.410	271.324
Na2O+	61.97839	506.227	517.290	520.834	57.404	14.607	280.689
Na2O2	77.97834	-139.496	-117.895	-123.930	68.503	15.565	289.595
Na2O2H2	79.99422	-643.346	-613.278	-624.000	97.360	19.346	309.772
Na2SO4	142.04214	-1061.104	-1026.412	-1040.132	105.223	20.972	345.365
Na3CL3	175.32831	-942.152	-909.000	-912.675	126.381	29.477	426.719
Na3F3	125.96452	-1373.618	-1341.000	-1348.015	119.035	25.602	372.029
Nb	92.90638	714.759	720.000	723.113	30.159	8.354	186.262
Nb+	92.90583	1385.016	1384.059	1393.605	30.291	8.589	182.978
Nb-	92.90693	622.400	633.839	631.054	28.948	8.654	186.097
NbCL5	270.17138	-729.673	-701.479	-703.330	119.042	26.343	404.118
NbO	108.90578	202.209	211.790	210.989	30.784	8.780	238.972
NbOCL3	215.26478	-772.931	-749.578	-752.300	92.002	20.631	358.302
NbO2	124.90518	-211.921	-198.000	-201.267	41.514	10.654	269.934
Ne	20.17970	-6.197	-6.197	0.000	20.786	6.197	146.330
Ne+	20.17915	2080.662	2080.662	2086.966	22.120	6.304	158.310
Ni	58.69340	423.292	428.078	430.117	23.361	6.825	182.193

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
Ni+	58.69285	1166.389	1164.977	1172.595	20.990	6.206	174.574
Ni-	58.69395	305.557	316.541	311.764	21.018	6.207	174.580
NiCL	94.14640	172.539	181.916	182.004	35.444	9.465	251.887
NiCL2	129.59940	-88.138	-74.170	-73.931	58.078	14.207	294.237
NiO	74.69280	288.197	297.323	297.064	31.701	8.867	231.090
NiS	90.75840	348.200	357.398	357.419	34.452	9.219	252.287
O	15.99940	242.450	246.790	249.175	21.912	6.725	161.060
O+	15.99885	1562.590	1560.732	1568.787	20.786	6.197	154.961
O-	15.99995	95.275	105.813	101.846	21.685	6.571	157.797
OD	18.01350	26.173	34.798	35.172	29.939	8.999	189.668
OD-	18.01405	-156.200	-141.378	-147.558	29.143	8.642	178.411
OH	17.00734	28.465	37.039	37.278	29.886	8.813	183.740
OH+	17.00679	1290.610	1292.987	1299.213	29.196	8.603	182.746
OH-	17.00789	-153.862	-139.091	-145.256	29.141	8.606	172.542
O2	31.99880	-8.680	-8.680	0.000	29.378	8.680	205.149
O2+	31.99825	1162.517	1165.000	1171.828	30.670	9.311	205.392
O2-	31.99935	-57.378	-42.500	-48.028	31.422	9.350	209.336
O3	47.99820	131.434	144.454	141.800	39.376	10.366	239.010
P	30.97376	310.303	315.663	316.500	20.786	6.197	163.200
P+	30.97321	1328.312	1327.474	1336.453	25.859	8.142	166.971
P-	30.97431	232.079	243.636	238.827	22.169	6.748	169.126
PCL	66.42676	125.324	135.275	134.615	33.991	9.291	236.883
PCL2	101.87976	-66.541	-52.000	-54.292	50.935	12.249	285.127
PCL2-	101.88031	-368.738	-348.000	-356.285	50.861	12.453	281.466
PCL3	137.33276	-305.432	-286.301	-289.500	71.592	15.932	311.708
PCL5	208.23876	-399.305	-370.993	-376.000	113.318	23.305	367.209
PF	49.97216	-56.836	-47.063	-47.945	31.619	8.891	225.006
PF+	49.97162	892.088	895.663	901.518	33.429	9.430	224.038
PF-	49.97271	-173.562	-157.592	-164.046	34.786	9.516	225.221
PFCL	85.42516	-294.815	-280.451	-283.184	47.535	11.630	279.494
PFCL-	85.42571	-541.012	-520.451	-529.269	47.800	11.743	274.544
PFCL2	120.87816	-526.793	-507.839	-511.925	67.435	14.868	307.925
PFCL4	191.78416	-656.750	-628.616	-635.016	107.850	21.734	358.036
PF2	68.97057	-524.185	-510.000	-513.104	44.304	11.081	262.183
PF2-	68.97112	-720.383	-700.000	-709.338	44.380	11.045	256.272
PF2CL	104.42357	-748.953	-730.177	-735.077	63.101	13.876	295.068
PF2CL3	175.32957	-898.910	-870.953	-878.745	102.183	20.165	338.132
PF3	87.96897	-970.336	-951.739	-957.400	58.685	12.936	273.060
PF3CL2	158.87497	-1141.070	-1113.291	-1122.023	97.348	19.047	335.435
PF4CL	142.42037	-1383.230	-1355.629	-1364.909	93.005	18.321	326.834
PF5	125.96578	-1609.838	-1582.415	-1593.300	84.703	16.538	301.026
PH	31.98170	222.104	231.698	230.752	29.175	8.648	196.381
PH2	32.98964	109.572	123.400	119.553	34.450	9.982	212.610
PH2-	32.99019	-19.226	0.800	-9.265	34.124	9.960	205.247
PH3	33.99758	-4.698	13.365	5.439	37.102	10.137	210.245
PN	44.98046	162.785	172.480	171.487	29.691	8.702	211.135
PO	46.97316	-37.248	-27.548	-27.858	31.761	9.390	222.744
PO-	46.97371	-148.845	-132.948	-140.067	30.759	8.778	222.403
POCL3	153.33216	-586.116	-562.644	-568.400	84.355	17.716	324.466
POFCL2	136.87756	-810.343	-787.050	-793.889	79.234	16.454	320.344
POF2CL	120.42297	-1037.503	-1014.388	-1022.607	73.066	14.896	305.054
POF3	103.96837	-1266.166	-1243.229	-1252.000	68.874	14.166	285.422
PO2	62.97256	-292.040	-278.000	-281.527	39.524	10.513	253.687
PO2-	62.97311	-608.237	-588.000	-597.624	40.517	10.614	249.406
PS	63.03876	140.815	150.587	150.431	35.242	9.616	234.068

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
P2	61.94752	135.096	145.816	144.000	32.032	8.904	218.124
P2O3	109.94572	-700.740	-677.000	-684.645	73.927	16.095	312.698
P2O4	125.94512	-951.080	-923.000	-933.755	85.131	17.326	312.913
P2O5	141.94452	-1146.420	-1114.000	-1124.370	105.936	22.050	366.580
P3	92.92128	197.994	214.074	210.000	51.873	12.006	263.529
P3O6	188.91768	-1599.120	-1557.000	-1575.681	135.741	23.439	376.077
P4	123.89504	44.791	66.231	58.900	67.081	14.109	279.883
P4O6	219.89144	-1630.798	-1583.317	-1606.000	148.611	24.798	356.395
P4O7	235.89084	-2010.820	-1959.000	-1984.448	159.256	26.372	379.867
P4O8	251.89024	-2330.160	-2274.000	-2302.214	169.902	27.946	394.949
P4O9	267.88964	-2643.500	-2583.000	-2613.979	180.548	29.521	402.497
P4O10	283.88904	-2937.320	-2872.479	-2906.223	191.196	31.097	402.094
Pb	207.20000	189.003	195.873	195.200	20.786	6.197	175.377
Pb+	207.19945	910.799	911.472	916.997	20.786	6.197	181.140
Pb-	207.20055	147.685	160.752	153.882	20.786	6.197	186.903
PbBr	287.10400	54.675	73.805	64.821	36.916	10.146	272.744
PbBr2	367.00800	-118.930	-87.540	-103.908	56.966	15.022	339.673
PbBr3	446.91200	-123.980	-80.330	-104.011	80.540	19.969	385.255
PbBr4	526.81600	-208.307	-152.397	-182.436	104.468	25.871	427.724
PbCL	242.65300	-0.968	10.493	8.819	36.215	9.787	261.306
PbCL2	278.10600	-189.550	-173.499	-175.547	55.299	14.003	315.621
PbCL3	313.55900	-195.909	-175.268	-177.654	77.918	18.256	351.604
PbCL4	349.01200	-350.880	-325.648	-327.430	100.537	23.449	381.682
PbF	226.19840	-108.136	-96.853	-98.868	34.401	9.268	249.962
PbF2	245.19681	-456.000	-440.305	-443.427	50.981	12.573	291.532
PbF3	264.19521	-505.108	-485.000	-489.573	70.582	15.535	316.287
PbF4	283.19361	-819.551	-795.031	-799.925	90.232	19.626	331.825
PbI	334.10447	98.565	112.033	108.904	37.152	10.339	280.413
PbI2	461.00894	-25.500	-5.434	-10.253	57.182	15.247	352.613
PbI3	587.91341	0.690	27.354	21.755	81.624	21.065	411.532
PbI4	714.81788	-68.747	-35.485	-41.226	106.254	27.521	463.806
PbO	223.19940	59.175	70.385	68.137	32.513	8.962	240.045
PbO2	239.19880	123.902	139.452	136.153	51.721	12.251	261.093
PbS	239.26500	118.515	129.797	127.945	35.085	9.430	251.414
PbS2	271.33000	230.028	245.722	244.049	57.511	14.021	286.141
Rb	85.46780	74.703	82.192	80.900	20.786	6.197	170.095
Rb+	85.46725	483.932	485.223	490.129	20.786	6.197	164.332
Rb-	85.46835	21.621	35.308	27.819	20.786	6.197	164.332
RbBO2	128.27760	-693.310	-675.927	-678.977	59.261	14.333	308.301
RbBr	165.37180	-201.830	-182.081	-191.511	37.217	10.319	261.132
RbCL	120.92080	-233.380	-221.300	-223.323	36.836	10.057	249.692
RbF	104.46620	-343.100	-331.198	-333.512	35.710	9.588	237.119
RbH	86.47574	110.504	122.227	119.324	31.305	8.820	208.726
RbI	212.37227	-148.940	-134.853	-138.481	37.372	10.459	268.872
RbK	124.56610	109.205	123.782	120.013	37.894	10.808	266.235
RbLi	92.40880	153.905	166.026	164.181	37.357	10.276	240.928
RbNO2	131.47330	-203.400	-182.896	-187.630	61.564	15.770	317.580
RbNO3	147.47270	-331.340	-306.496	-314.972	68.981	16.368	326.440
RbNa	108.45757	120.805	134.754	131.470	37.879	10.665	256.435
RbO	101.46720	42.152	53.981	52.489	42.496	10.337	244.913
RbOH	102.47514	-249.761	-233.698	-238.000	49.520	11.761	248.502
Rb2Br2	330.74360	-573.498	-534.000	-551.801	82.195	21.697	398.376
Rb2CL2	241.84160	-639.159	-615.000	-618.374	81.442	20.786	374.474
Rb2F2	208.93241	-873.803	-850.000	-854.913	79.075	18.890	342.830
Rb2I2	424.74454	-455.174	-427.000	-432.956	82.508	22.218	416.286

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
Rb2O	186.93500	-123.145	-103.827	-108.929	54.827	14.216	307.147
Rb2O2	202.93440	-232.696	-209.037	-215.848	71.934	16.847	326.309
Rb2O2H2	204.95028	-662.407	-630.281	-639.000	107.351	23.407	367.188
Rb2SO4	266.99820	-1119.914	-1083.164	-1096.592	109.390	23.322	392.360
Rn	222.01760	-6.197	-6.197	0.000	20.786	6.197	176.238
Rn+	222.01705	1037.073	1037.073	1043.270	20.786	6.197	187.764
S	32.06500	270.513	274.925	277.170	23.674	6.657	167.832
S+	32.06445	1276.299	1274.514	1282.496	20.786	6.197	163.631
S-	32.06555	63.904	74.513	70.369	22.783	6.465	164.923
SCL	67.51800	146.646	155.648	156.465	37.542	9.819	237.328
SCL2	102.97100	-30.018	-16.425	-17.573	50.896	12.445	281.632
SCL2+	102.97045	888.930	896.326	901.383	50.861	12.453	287.326
SD	34.07910	129.196	137.893	138.491	32.520	9.294	201.488
SF	51.06340	5.975	14.800	15.446	35.180	9.470	225.281
SF+	51.06285	985.706	988.333	994.570	31.679	8.864	225.410
SF-	51.06395	-240.222	-225.200	-231.347	31.787	8.875	216.350
SF2	70.06181	-304.237	-291.000	-293.189	44.415	11.048	256.582
SF2+	70.06126	694.782	701.821	706.016	44.937	11.234	263.528
SF2-	70.06235	-406.920	-387.485	-394.795	50.165	12.125	267.450
SF3	89.06021	-517.650	-500.000	-504.101	63.148	13.548	285.616
SF3+	89.05966	381.174	392.627	393.583	56.224	12.409	268.976
SF3-	89.06076	-803.847	-780.000	-790.124	64.068	13.723	281.593
SF4	108.05861	-775.383	-753.321	-760.000	76.673	15.383	296.713
SF4+	108.05806	399.606	415.471	416.112	80.396	16.506	311.676
SF4-	108.05916	-905.945	-877.685	-887.464	89.189	18.480	312.967
SF5	127.05702	-921.475	-895.000	-902.663	100.085	18.811	322.275
SF5+	127.05647	156.297	176.574	172.644	89.844	16.347	298.156
SF5-	127.05756	-1223.672	-1191.000	-1204.622	101.065	19.050	317.070
SF6	146.05542	-1236.340	-1205.453	-1219.400	97.069	16.940	291.678
SF6-	146.05597	-1359.367	-1322.282	-1341.876	99.986	17.491	302.865
SH	33.07294	133.037	141.683	142.135	32.479	9.098	195.554
SH-	33.07349	-95.220	-80.377	-86.574	29.146	8.646	186.638
SN	46.07170	257.995	266.742	267.388	31.795	9.393	222.095
SO	48.06440	-4.038	4.714	4.760	30.176	8.798	221.941
SO-	48.06495	-115.435	-100.486	-105.968	34.425	9.467	223.678
SOF2	86.06121	-597.577	-580.000	-584.952	57.095	12.625	279.138
SO2	64.06380	-307.358	-294.266	-296.810	39.842	10.548	248.222
SO2-	64.06435	-419.356	-400.066	-408.606	41.795	10.749	256.027
SO2CL2	134.96980	-370.832	-348.559	-354.803	77.096	16.029	311.101
SO2FCL	118.51520	-571.173	-549.078	-556.472	71.593	14.701	302.854
SO2F2	102.06061	-773.490	-751.573	-760.000	65.776	13.490	283.543
SO3	80.06320	-407.588	-390.156	-395.900	50.619	11.688	256.547
S2	64.13000	119.468	128.292	128.600	32.505	9.132	228.166
S2-	64.13055	-46.730	-31.708	-37.132	37.193	9.597	228.429
S2CL2	135.03600	-33.257	-15.252	-16.736	72.776	16.521	327.237
S2F2	102.12681	-415.131	-397.482	-401.413	63.128	13.718	292.832
S2O	80.12940	-67.164	-54.000	-56.035	44.114	11.129	266.967
S3	96.19500	132.764	146.000	144.738	48.964	11.974	276.296
S4	128.26000	121.352	139.000	135.632	65.944	14.280	293.565
S5	160.32500	113.940	136.000	132.993	87.870	19.053	354.086
S6	192.39000	78.528	105.000	101.315	113.155	22.787	357.812
S7	224.45500	85.616	116.500	111.890	133.866	26.274	404.855
S8	256.52000	69.704	105.000	101.277	156.503	31.573	432.545
Sc	44.95591	370.698	375.905	377.700	22.103	7.002	174.788
Sc+	44.95536	1009.983	1008.993	1017.145	21.762	7.162	178.338

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
Sc-	44.95646	346.361	357.766	352.559	20.786	6.197	187.196
ScO	60.95531	-63.852	-54.305	-55.065	30.864	8.787	224.550
ScO+	60.95476	552.433	555.783	561.210	30.744	8.777	218.504
ScO2	76.95471	-424.403	-410.516	-413.651	42.467	10.752	262.583
Sc2O	105.91122	-34.754	-20.000	-23.044	46.529	11.710	270.389
Sc2O2	121.91062	-503.705	-484.611	-490.571	56.093	13.134	283.193
Si	28.08550	442.450	445.667	450.000	22.251	7.550	167.982
Si+	28.08495	1235.165	1232.185	1242.508	24.336	7.343	163.429
Si-	28.08605	302.620	312.035	308.818	20.786	6.197	161.979
SiBr	107.98950	165.122	180.600	175.157	38.711	10.035	247.288
SiBr2	187.89350	-64.317	-36.580	-51.000	53.588	13.317	304.721
SiBr3	267.79750	-174.461	-134.464	-157.000	75.234	17.461	351.326
SiBr4	347.70150	-438.114	-385.856	-415.800	97.010	22.314	379.375
SiC	40.09620	725.729	730.000	734.946	31.032	9.217	226.213
SiC2	52.10690	619.676	625.000	631.361	44.227	11.685	252.239
SiCL	63.53850	132.479	140.287	142.363	35.783	9.884	237.840
SiCL2	98.99150	-175.599	-163.200	-163.069	51.274	12.529	281.618
SiCL3	134.44450	-351.989	-335.000	-336.272	70.563	15.717	316.646
SiCL4	169.89750	-681.655	-660.076	-662.200	90.406	19.455	331.452
SiF	47.08390	-34.689	-27.059	-25.233	32.653	9.456	225.790
SiFCL	82.53690	-389.659	-377.439	-377.827	47.494	11.833	275.147
SiF2	66.08231	-604.043	-592.000	-592.838	44.510	11.204	256.588
SiF3	85.08071	-1009.455	-993.000	-996.437	58.730	13.019	279.708
SiF4	104.07911	-1631.146	-1610.278	-1615.780	73.753	15.366	282.810
SiH	29.09344	359.491	366.943	368.636	30.054	9.145	198.054
SiH+	29.09289	1139.017	1140.271	1147.671	29.184	8.654	186.791
SiHBr3	268.80544	-320.745	-276.514	-302.922	80.411	17.823	348.054
SiHCL	64.54644	44.281	56.323	54.946	41.015	10.665	251.334
SiHCL3	135.45244	-512.374	-491.150	-496.222	75.457	16.152	313.722
SiHF	48.09184	-172.887	-161.023	-162.657	37.793	10.230	238.693
SiHF3	86.08865	-1214.353	-1193.663	-1200.808	63.486	13.545	277.272
SiHI3	409.80685	-93.610	-66.365	-74.475	83.886	19.135	375.011
SiH2	30.10138	263.314	275.000	273.333	34.973	10.018	207.483
SiH2Br2	189.90938	-204.644	-168.439	-190.372	65.546	14.272	310.056
SiH2CL2	101.00738	-333.879	-313.012	-320.494	62.175	13.385	286.738
SiH2F2	68.09819	-802.764	-782.254	-790.776	54.269	11.988	262.134
SiH2I2	283.91032	-52.991	-28.110	-38.074	67.981	14.917	326.801
SiH3	31.10932	194.080	210.000	204.357	38.920	10.277	216.498
SiH3Br	111.01332	-90.010	-61.831	-78.241	52.866	11.769	262.470
SiH3CL	66.56232	-153.279	-132.769	-141.838	51.099	11.441	250.765
SiH3F	50.10772	-387.492	-367.159	-376.560	47.197	10.932	238.405
SiH3I	158.01379	-14.170	8.347	-2.092	54.402	12.078	271.026
SiH4	32.11726	24.165	44.319	34.700	42.787	10.535	204.208
SiI	154.98997	253.012	262.828	262.953	39.009	9.941	253.881
SiI2	281.89444	78.673	95.087	92.466	54.625	13.793	320.976
SiN	42.09220	394.932	402.485	403.668	30.281	8.736	216.814
SiO	44.08490	-107.558	-100.000	-98.842	29.901	8.715	211.600
SiO2	60.08430	-332.616	-320.718	-322.073	44.055	10.543	228.724
SiS	60.15050	99.262	106.892	108.194	32.273	8.932	223.675
SiS2	92.21550	-5.181	6.861	7.023	51.814	12.203	254.063
Si2	56.17100	569.899	576.334	580.196	36.265	10.296	238.007
Si2C	68.18170	542.512	550.000	554.094	45.336	11.582	261.900
Si2F6	170.16142	-2409.984	-2377.074	-2383.290	129.879	26.694	391.386
Si2N	70.17770	385.658	396.428	397.480	49.885	11.822	256.491
Si3	84.25650	615.348	625.000	627.867	50.959	12.520	279.184

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	T = 298.15 K: $C_p^o(T)$ J/K-mol	T = 298.15 K: $H^o(T) - H^o(0)$ kJ/mol	T = 298.15 K: $S^o(T)$ J/K-mol
Sn	118.71000	294.985	301.308	301.200	21.260	6.215	168.495
Sn+	118.70945	1009.753	1009.878	1015.950	20.786	6.197	174.193
Sn-	118.71055	173.006	185.526	179.496	24.464	6.490	181.197
SnBr	198.61400	65.658	84.241	75.644	36.648	9.986	264.831
SnBr2	278.51800	-133.570	-102.727	-118.975	56.392	14.595	329.048
SnBr3	358.42200	-177.997	-134.894	-158.716	79.523	19.280	373.603
SnBr4	438.32600	-349.260	-293.897	-324.217	103.285	25.043	413.236
SnCL	154.16300	25.015	35.928	34.659	35.836	9.644	253.414
SnCL2	189.61600	-216.330	-200.826	-202.648	54.636	13.682	305.905
SnCL3	225.06900	-309.926	-289.832	-292.372	76.331	17.554	339.854
SnCL4	260.52200	-500.940	-476.255	-478.466	98.401	22.474	366.879
SnF	137.70840	-104.153	-93.418	-95.017	33.701	9.136	241.615
SnF2	156.70681	-523.200	-508.052	-510.957	49.680	12.243	282.130
SnF3	175.70521	-661.430	-641.870	-646.630	67.799	14.800	304.054
SnF4	194.70361	-1043.569	-1019.595	-1024.767	86.601	18.802	319.474
SnI	245.61447	162.548	175.469	172.725	36.986	10.177	272.297
SnI2	372.51894	-22.950	-3.431	-8.067	56.744	14.883	342.708
SnI3	499.42341	-28.327	-2.210	-8.018	80.792	20.309	398.029
SnI4	626.32788	-145.600	-112.885	-118.854	105.468	26.746	448.738
SnO	134.70940	13.037	23.700	21.911	31.761	8.874	232.118
SnO2	150.70880	-0.116	14.888	11.680	49.548	11.796	251.613
SnS	150.77500	101.798	112.533	111.099	34.537	9.301	243.578
SnS2	182.84000	136.011	151.158	149.646	56.436	13.635	277.046
Sn2	237.42000	409.971	422.617	421.344	42.114	11.373	267.314
Sr	87.62000	154.303	160.861	160.500	20.786	6.197	164.642
Sr+	87.61945	709.969	710.330	716.166	20.786	6.197	170.405
SrBr	167.52400	-74.025	-55.207	-63.918	36.865	10.107	263.877
SrBr2	247.42800	-423.060	-391.982	-406.726	61.239	16.335	326.410
SrCL	123.07300	-137.668	-126.519	-127.868	36.260	9.800	252.470
SrCL+	123.07245	398.529	403.481	408.112	35.621	9.583	244.740
SrCL2	158.52600	-499.230	-483.491	-484.814	55.767	14.416	314.932
SrF	106.61840	-312.836	-301.865	-303.553	34.473	9.283	239.903
SrF+	106.61785	200.362	205.135	209.468	33.509	9.107	232.600
SrF2	125.61681	-798.063	-782.680	-784.794	52.785	13.270	290.677
SrH	88.62794	210.504	221.296	219.227	30.133	8.723	212.753
SrI	214.52447	-18.135	-4.979	-7.852	37.103	10.283	271.890
SrI2	341.42894	-294.921	-275.166	-278.219	61.595	16.702	341.645
SrO	103.61940	-23.248	-12.349	-14.208	33.089	9.040	230.057
SrO+	103.61885	619.950	624.651	630.054	35.190	10.104	244.840
SrOH	104.62734	-205.132	-190.000	-194.086	47.064	11.047	248.661
SrOH+	104.62679	299.065	308.000	310.170	47.341	11.105	243.763
Sr(OH)2	121.63468	-613.706	-590.000	-596.695	78.877	17.012	309.408
SrS	119.68500	94.815	105.785	104.351	35.480	9.536	243.111
Sr2	175.24000	296.205	309.322	307.570	36.516	11.365	278.279
Ta	180.94790	776.319	782.000	782.519	20.858	6.200	185.221
Ta+	180.94735	1543.341	1542.825	1549.679	23.109	6.338	183.387
Ta-	180.94845	739.053	750.932	745.469	24.561	6.416	174.563
TaCL5	358.21290	-791.704	-763.070	-764.835	120.139	26.869	412.979
TaO	196.94730	233.769	243.790	242.535	30.600	8.766	241.118
TaO2	212.94670	-184.361	-170.000	-173.662	41.795	10.699	277.388
Ti	47.86700	465.461	470.285	473.000	24.430	7.539	180.296
Ti+	47.86645	1129.724	1128.351	1137.624	26.186	7.900	183.591
Ti-	47.86755	451.641	462.663	459.204	22.835	7.563	183.714
TiCL	83.32000	141.170	150.585	150.851	37.300	9.681	249.219
TiCL2	118.77300	-250.775	-236.770	-237.230	57.504	13.545	278.340

Appendix B (*continued*)

TABLE B1 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
TiCL3	154.22600	-554.695	-536.099	-539.320	72.568	15.375	316.898
TiCL4	189.67900	-784.774	-761.587	-763.160	95.615	21.614	354.894
TiO	63.86640	39.910	49.075	49.504	31.880	9.593	233.267
TiO+	63.86585	676.108	679.075	685.321	30.941	9.213	229.839
TiOCL	99.31940	-256.405	-242.650	-244.262	51.655	12.143	263.663
TiOCL2	134.77240	-562.262	-543.917	-545.552	71.953	16.710	321.005
TiO2	79.86580	-316.782	-303.278	-305.430	44.087	11.352	260.127
U	238.02891	528.501	534.865	535.000	23.694	6.499	199.790
UF	257.02731	-58.638	-47.861	-49.251	37.949	9.387	251.805
UF+	257.02676	547.560	552.139	557.059	40.248	9.499	251.850
UF-	257.02786	-164.835	-147.861	-155.679	33.802	9.156	250.918
UF2	276.02572	-550.189	-535.000	-535.037	56.172	15.152	315.812
UF2+	276.02517	56.008	65.000	70.446	55.395	14.437	313.999
UF2-	276.02627	-691.387	-670.000	-678.233	55.900	13.153	303.914
UF3	295.02412	-1079.602	-1060.000	-1060.959	76.183	18.643	347.433
UF3+	295.02357	-303.404	-290.000	-284.745	81.735	18.659	338.293
UF3-	295.02467	-1205.799	-1180.000	-1186.441	76.960	19.358	349.245
UF4	314.02252	-1628.050	-1604.036	-1606.157	101.356	21.893	363.179
UF4+	314.02197	-661.853	-644.036	-641.539	91.910	20.313	361.099
UF4-	314.02307	-1750.212	-1720.000	-1728.335	95.803	21.877	372.319
UF5	333.02093	-1973.427	-1945.000	-1949.824	110.637	23.603	386.344
UF5+	333.02038	-877.229	-855.000	-853.617	110.650	23.612	380.630
UF5-	333.02147	-2314.624	-2280.000	-2289.431	120.145	25.193	388.479
UF6	352.01933	-2175.265	-2142.426	-2148.642	129.499	26.623	376.690
UF6-	352.01988	-2719.037	-2680.000	-2691.306	132.268	27.731	392.875
UO	254.02831	20.950	31.654	30.489	42.001	9.538	248.870
UO+	254.02776	572.148	576.654	580.972	31.303	8.824	245.711
UOF	273.02671	-556.188	-541.072	-542.183	53.474	14.005	313.309
UOF2	292.02512	-1133.327	-1113.798	-1115.510	79.293	17.816	336.615
UOF3	311.02352	-1530.465	-1506.523	-1510.638	89.110	19.827	353.073
UOF4	330.02192	-1808.354	-1780.000	-1785.612	108.119	22.743	363.175
UO2	270.02771	-491.280	-476.236	-477.820	59.546	13.460	266.428
UO2+	270.02716	39.917	48.764	51.494	48.698	11.577	261.758
UO2-	270.02826	-587.477	-566.236	-573.700	55.379	13.777	278.453
UO2F	289.02611	-1013.739	-994.282	-997.935	67.978	15.804	328.807
UO2F2	308.02452	-1373.300	-1349.431	-1354.232	86.386	19.068	342.636
UO3	286.02711	-814.384	-795.000	-799.239	64.530	15.145	309.647
UO3-	286.02766	-1320.582	-1295.000	-1305.155	66.105	15.427	318.297
V	50.94150	509.360	514.000	517.267	26.012	7.907	182.301
V+	50.94095	1165.848	1164.290	1173.745	23.150	7.898	183.378
V-	50.94205	452.508	463.345	460.386	23.049	7.878	183.438
VCL4	192.75350	-548.842	-525.839	-527.058	96.045	21.783	366.518
VN	64.94820	514.200	523.175	523.000	31.148	8.800	233.387
VO	66.94090	139.810	148.790	148.583	30.698	8.773	230.903
VO2	82.94030	-243.320	-230.000	-232.698	41.223	10.622	261.997
V4O10	363.76000	-2861.961	-2800.000	-2825.164	218.472	36.796	445.617
W	183.84000	845.027	850.000	851.244	21.306	6.217	173.957
W+	183.83945	1621.620	1620.395	1627.841	21.372	6.221	179.739
W-	183.84055	760.194	771.365	766.392	20.786	6.197	188.782
WCL6	396.55800	-524.503	-491.987	-493.712	143.943	30.791	419.172
WO	199.83940	392.477	401.790	401.736	30.698	9.259	244.227
WOCL4	341.65140	-595.764	-568.089	-573.493	106.140	22.271	377.085
WO2	215.83880	18.347	32.000	29.062	41.980	10.715	271.487
WO2CL2	286.74480	-691.036	-668.202	-671.532	87.200	19.504	353.932
WO3	231.83820	-332.993	-315.000	-319.725	59.164	13.268	283.127

Appendix B (*continued*)

TABLE B1 (*concluded*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
WO3-	231.83875	-664.191	-640.000	-650.476	61.174	13.715	291.664
(WO3)2	463.67640	-1235.986	-1200.000	-1210.443	128.395	25.543	395.245
(WO3)3	695.51460	-2053.979	-2000.000	-2013.291	204.304	40.688	518.322
(WO3)4	927.35280	-2871.973	-2800.000	-2817.434	276.407	54.539	618.888
(WO3)5	1159.19100	-3619.966	-3530.000	-3551.492	349.313	68.473	717.875
Xe	131.29300	-6.197	-6.197	0.000	20.786	6.197	169.686
Xe+	131.29245	1170.355	1170.355	1176.552	20.786	6.197	181.213
Zn	65.39000	124.203	129.860	130.400	20.786	6.197	160.993
Zn+	65.38945	1036.803	1036.262	1043.000	20.786	6.197	166.756
Zr	91.22400	592.503	598.000	599.319	26.642	6.816	181.346
Zr+	91.22345	1238.774	1238.074	1246.246	28.283	7.472	183.642
Zr-	91.22455	545.203	556.897	552.952	28.693	7.749	185.765
ZrN	105.23070	704.509	714.341	713.372	31.661	8.863	233.491
ZrO	107.22340	74.953	84.790	83.923	34.374	8.970	228.187
ZrO+	107.22285	711.150	714.790	720.614	33.471	9.464	236.915
ZrO2	123.22280	-329.051	-314.874	-317.043	46.062	12.008	273.750
Air	28.96512	-8.775	-0.125	-0.126	29.102	8.649	198.822
CLO3F	102.44960	-37.099	-15.076	-23.800	64.925	13.299	278.989
JP-10(g)	136.23404	-109.853	-31.574	-86.856	152.560	22.997	359.201
Jet-A(g)	167.31102	(a)	(a)	-249.657	293.491	(a)	628.437

[a] No data available for 0 K.

Appendix B (*continued*)

TABLE B2.—THERMODYNAMIC PROPERTIES FOR CONDENSED SPECIES AT 0 AND 298.15 K

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	T = 298.15 K: $C_p^o(T)$ J/K-mol	T = 298.15 K: $H^o(T) - H^o(0)$ kJ/mol	T = 298.15 K: $S^o(T)$ J/K-mol
Ag(cr)	107.86820	-5.745	-5.745	0.000	25.350	5.745	42.550
AL(cr)	26.98154	-4.540	-4.540	0.000	24.200	4.540	28.300
ALBr3(cr)	266.69354	-533.420	-492.100	-511.500	100.562	21.920	180.250
ALCL3(cr)	133.33964	-722.080	-703.768	-705.100	91.133	16.980	109.290
ALF3(II)	83.97675	-1522.020	-1504.243	-1510.400	75.122	11.620	66.500
ALH3(a)	30.00536	-16.840	0.402	-11.400	40.210	5.440	30.040
ALI3(cr)	407.69495	-325.200	-300.866	-302.900	98.893	22.300	190.000
ALN(cr)	40.98828	-322.870	-313.995	-319.000	30.087	3.870	20.170
AL(OH)3(a)	78.00356	-1305.960	-1275.698	-1293.500	91.969	12.460	68.440
AL2O3(a)	101.96128	-1685.716	-1663.616	-1675.700	79.033	10.016	50.920
AL2S3(a)	150.16108	-667.130	-644.814	-648.500	105.060	18.630	116.860
AL2SiO5(an)	162.04558	-2609.165	-2575.167	-2592.072	122.755	17.093	93.221
AL4C3(cr)	143.95825	-223.370	-202.049	-206.900	116.779	16.470	88.950
B(b)	10.81100	-1.214	-1.214	0.000	11.315	1.214	5.834
BN(cr)	24.81774	-253.628	-248.079	-251.000	19.705	2.628	14.810
B2O3(cr)	69.62020	-1282.801	-1267.353	-1273.500	62.761	9.301	53.970
B2S3(cr)	117.82000	-260.200	-244.536	-243.000	111.724	17.200	100.000
B3O3H3(cr)	83.45502	(a)	(a)	-1262.313	98.324	(a)	167.360
B4C(cr)	55.25470	-67.611	-61.702	-62.000	53.090	5.611	27.110
Ba(cr)	137.32700	-6.907	-6.907	0.000	28.110	6.907	62.352
BaBr2(cr)	297.13500	-771.000	-739.573	-752.000	75.942	19.000	150.000
BaCO3(a)	197.33590	-1230.510	-1209.530	-1214.000	85.983	16.510	112.100
BaCL2(a)	208.23240	-871.900	-855.812	-855.200	75.140	16.700	123.700
BaF2(a)	175.32381	-1220.440	-1204.708	-1206.000	71.129	14.440	96.360
BaH2(a)	139.34288	-199.100	-183.725	-190.000	46.000	9.100	63.000
BaI2(cr)	391.13594	-625.230	-605.127	-606.000	77.488	19.230	165.200
BaO(cr)	153.32640	-557.962	-546.715	-548.000	47.020	9.962	72.000
Ba(OH)2(b)	171.34168	-956.748	-932.693	-940.600	89.080	16.148	107.280
BaS(cr)	169.39300	-480.820	-469.501	-470.000	49.370	10.820	78.450
BaSO4(a)	233.39060	-1489.180	-1460.501	-1470.000	102.096	19.180	132.100
Be(a)	9.01218	-1.942	-1.942	0.000	16.443	1.942	9.503
BeAL2O4(cr)	126.97286	-2313.870	-2285.488	-2300.782	105.380	13.088	66.291
BeBr2(cr)	168.82018	-372.900	-346.438	-358.000	69.454	14.900	108.000
BeCO3(cr)	69.02108	-1054.200	-1038.185	-1045.000	64.995	9.200	52.000
BeCL2(a)	79.91758	-507.620	-496.497	-496.200	62.421	11.420	75.810
BeF2(a)	47.00899	-1035.468	-1024.701	-1027.000	51.840	8.468	53.350
BeI2(cr)	262.82112	-206.200	-191.062	-191.000	71.128	15.200	121.000
BeO(a)	25.01158	-612.237	-605.955	-609.400	25.565	2.837	13.770
Be(OH)2(b)	43.02686	-913.993	-894.903	-905.700	62.132	8.293	45.480
BeS(cr)	41.07818	-241.500	-235.146	-236.000	33.998	5.500	34.000
BeSO4(a)	105.07578	-1212.970	-1189.256	-1200.000	85.689	12.970	77.910
Be2C(cr)	30.03506	(a)	(a)	-116.985	43.264	(a)	16.318
Be3N2(a)	55.05003	-595.124	-580.628	-588.000	64.757	7.124	34.400
Br2(cr)	159.80800	-24.520	-24.520	0.000	75.680	24.520	152.210
C(gr)	12.01070	-1.054	-1.054	0.000	8.528	1.054	5.734
Ca(a)	40.07800	-5.783	-5.783	0.000	25.750	5.783	42.536
CaBr2(cr)	199.88600	-700.800	-670.498	-683.800	75.061	17.000	130.000
CaCO3(cr)	100.08690	-1221.080	-1201.224	-1206.600	83.472	14.480	91.710
CaCL2(cr)	110.98340	-811.100	-796.136	-795.800	72.846	15.300	108.400
CaF2(a)	78.07481	-1239.640	-1225.032	-1228.000	67.027	11.640	68.450

Appendix B (*continued*)

TABLE B2 (*continued*)

Species name	Molecular weight	$H^\circ(0)$ kJ/mol	$\Delta_f H^\circ(0)$ kJ/mol	$T = 298.15$ K: $\Delta_f H^\circ(T)$ kJ/mol	$T = 298.15$ K: $C_p^\circ(T)$ J/K-mol	$T = 298.15$ K: $H^\circ(T) - H^\circ(0)$ kJ/mol	$T = 298.15$ K: $S^\circ(T)$ J/K-mol
CaH2(a)	42.09388	-183.770	-169.519	-177.000	41.000	6.770	41.400
CaI2(cr)	293.88694	-554.370	-535.392	-536.400	76.986	17.970	145.300
CaO(cr)	56.07740	-641.670	-631.548	-634.920	42.050	6.751	38.100
Ca(OH)2(cr)	74.09268	-1000.060	-977.129	-985.900	87.488	14.160	83.400
CaS(cr)	72.14400	-484.010	-473.816	-475.000	47.449	9.010	56.500
CaSO4(II)	136.14160	-1451.200	-1423.645	-1434.000	99.660	17.201	107.000
Cd(cr)	112.41100	-6.247	-6.247	0.000	26.020	6.247	51.800
Co(a)	58.93320	-4.771	-4.771	0.000	24.802	4.771	30.067
Cr(cr)	51.99610	-4.057	-4.057	0.000	23.434	4.057	23.618
CrN(cr)	66.00284	-124.857	-116.465	-117.152	52.677	7.705	37.711
Cr2N(cr)	117.99894	(a)	(a)	-125.520	66.065	(a)	64.852
Cr2O3(I')	151.99040	-1155.900	-1134.766	-1140.600	120.080	15.300	81.100
Cs(cr)	132.90545	-7.711	-7.711	0.000	32.210	7.711	85.230
CsBO2(cr)	175.71525	-976.368	-958.763	-962.000	80.580	14.368	104.350
CsBr(cr)	212.80945	-418.735	-398.764	-405.600	52.930	13.135	112.940
CsCL(a)	168.35815	-454.760	-442.458	-442.310	52.470	12.450	101.170
CsF(cr)	151.90385	-568.860	-556.736	-557.100	51.090	11.760	92.960
CsH(cr)	133.91339	-64.540	-52.595	-54.040	40.600	10.500	73.000
CsI(cr)	259.80992	-361.570	-347.261	-348.100	52.470	13.470	122.200
CsNO2(I)	178.91099	-403.320	-382.594	-379.900	91.340	23.420	174.000
CsNO3(a)	194.91039	-525.050	-499.984	-505.000	96.140	20.050	153.830
CsOH(b)	149.91279	-430.303	-414.018	-416.200	69.930	14.103	104.220
CsO2(a)	164.90425	-304.100	-287.709	-286.100	79.000	18.000	142.000
Cs2CO3(cr)	325.81980	-1160.627	-1131.131	-1134.900	123.850	25.727	204.470
Cs2O(cr)	281.81030	-364.080	-344.318	-346.400	76.000	17.680	146.900
Cs2O2(cr)	297.80970	-461.300	-437.198	-440.000	95.000	21.300	180.000
Cs2SO4(a)	361.87450	-1470.640	-1433.446	-1442.900	134.892	27.740	211.910
Cu(cr)	63.54600	-5.004	-5.004	0.000	24.440	5.004	33.150
CuBr(a)	143.45000	(a)	(a)	-105.604	54.743	(a)	96.102
CuBr2(cr)	223.35400	(a)	(a)	-138.490	75.740	(a)	128.867
CuCL(a)	98.99870	(a)	(a)	-155.645	52.534	(a)	87.743
CuCL2(cr)	134.45140	(a)	(a)	-217.986	71.873	(a)	108.073
CuF(cr)	82.54440	(a)	(a)	-209.200	51.882	(a)	64.852
CuF2(cr)	101.54281	(a)	(a)	-539.820	66.162	(a)	78.032
CuI(a)	190.45047	-79.960	-68.358	-67.781	54.057	12.180	96.596
CuO(cr)	79.54540	-162.745	-153.401	-155.645	42.296	7.100	42.635
Cu(OH)2(cr)	97.56068	(a)	(a)	-443.086	87.864	(a)	87.027
CuS(cr)	95.61200	(a)	(a)	-55.647	47.380	(a)	67.166
CuSO4(cr)	159.60960	-785.471	-758.694	-768.601	98.876	16.870	109.508
Cu2O(cr)	143.09140	-183.305	-168.957	-170.707	62.593	12.598	92.395
Cu2S(a)	159.15800	(a)	(a)	-75.730	76.910	(a)	116.152
Fe(a)	55.84500	-4.507	-4.507	0.000	25.094	4.507	27.321
Fe(CO)5(L)	195.89550	-819.024	-787.550	-766.090	233.785	52.934	337.078
FeCL2(cr)	126.75040	-358.106	-344.418	-341.833	76.664	16.273	117.947
FeCL3(cr)	162.20310	-418.678	-400.399	-399.237	96.943	19.441	147.821
Fe.947O(cr)	68.88461	(a)	(a)	-266.270	47.990	(a)	57.488
FeOCL(cr)	107.29710	-423.935	-410.497	-410.994	70.501	12.940	82.551
Fe(OH)2(cr)	89.85968	(a)	(a)	-574.045	97.069	(a)	87.864
Fe(OH)3(cr)	106.86702	(a)	(a)	-832.616	101.671	(a)	104.600
FeS(a)	87.91100	-109.035	-100.116	-99.621	50.543	9.414	60.312
FeSO4(cr)	151.90860	-945.617	-919.338	-928.848	100.583	16.769	120.955
FeS2(cr)	119.97700	-181.185	-167.854	-171.544	62.124	9.641	52.915
Fe2O3(cr)	159.68820	(a)	(a)	-824.248	103.763	(a)	87.404
Fe2(SO4)3(cr)	399.88080	(a)	(a)	-2582.992	264.722	(a)	307.524
Fe3O4(cr)	231.53260	-1143.145	-1112.264	-1118.383	150.791	24.762	146.147

Appendix B (*continued*)

TABLE B2 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
Ga(cr)	69.72300	-5.640	-5.640	0.000	26.099	5.640	41.220
GaBr3(cr)	309.43500	-412.000	-369.580	-387.000	99.000	25.000	180.000
GaCL3(cr)	176.08110	-547.000	-527.588	-527.000	96.000	20.000	134.000
GaF3(cr)	126.71821	-1191.700	-1172.822	-1175.000	89.000	16.700	96.000
GaI3(cr)	450.43641	-247.000	-221.566	-218.000	100.000	29.000	205.000
Ga2O3(cr)	187.44420	-1105.550	-1081.250	-1091.000	92.131	14.550	84.940
Ge(cr)	72.61000	-4.636	-4.636	0.000	23.222	4.636	31.090
GeO2(II)	104.60880	-587.430	-574.114	-580.200	50.166	7.230	39.710
GeS(cr)	104.67600	-85.005	-75.957	-75.348	47.782	9.657	66.480
GeS2(II)	136.74200	-134.250	-120.790	-121.500	65.700	12.750	93.600
HBO2(cr)	43.81774	-813.060	-798.932	-804.600	54.706	8.460	49.000
H2O(cr)	18.01528	(a)	(a)	-292.727	41.977	(a)	44.827
H2O(L)	18.01528	-299.108	-286.300	-285.830	75.351	13.278	69.942
H2SO4(L)	98.07948	-842.215	-811.975	-813.989	138.584	28.226	156.895
H3BO3(cr)	61.83302	-1108.320	-1081.384	-1094.800	86.060	13.520	89.950
H3PO4(cr)	97.99518	-1301.468	-1266.046	-1284.488	106.064	16.980	110.544
Hg(cr)	200.59000	-9.343	-9.343	0.001	27.975	9.344	76.030
HgBr2(cr)	360.39800	(a)	(a)	-175.310	75.312	(a)	170.314
HgO(cr)	216.58940	-99.893	-86.210	-90.789	44.062	9.104	70.270
I2(cr)	253.80894	-13.196	-13.196	0.000	54.440	13.196	116.139
In(cr)	114.81800	-6.610	-6.610	0.000	26.900	6.610	57.651
InBr(cr)	194.72200	-187.200	-168.330	-175.000	50.000	12.200	110.000
InBr3(cr)	354.53000	-423.500	-380.110	-399.000	102.000	24.500	175.000
InCL(crII)	150.27070	-198.900	-187.699	-186.500	51.460	12.400	100.000
InCl3(cr)	221.17610	-551.000	-530.618	-530.000	100.000	21.000	142.000
InF3(cr)	171.81321	-1209.400	-1189.552	-1190.000	91.999	19.400	110.000
InI(cr)	241.72247	-115.854	-102.646	-102.500	52.789	13.354	120.100
InI2(crII)	368.62694	-195.197	-175.391	-176.000	77.320	19.197	173.900
InI3(cr)	495.53141	-253.888	-227.484	-224.000	102.900	29.888	223.100
In2O3(cr)	277.63420	-939.600	-913.360	-923.000	99.070	16.600	101.800
K(cr)	39.09830	-7.088	-7.088	0.000	29.600	7.088	64.680
KALO2(II)	98.07864	-1143.955	-1123.647	-1130.600	76.120	13.355	85.550
KBO2(cr)	81.90810	-995.114	-978.132	-983.000	67.030	12.114	80.000
KBr(cr)	119.00230	-405.660	-386.312	-393.450	52.470	12.210	95.920
KCN(II)	65.11574	-130.813	-118.336	-113.470	66.391	17.343	127.780
KCL(cr)	74.55100	-447.860	-436.181	-436.490	51.300	11.370	82.570
KF(cr)	58.09670	-579.900	-568.399	-569.900	48.990	10.000	66.500
KH(cr)	40.10624	-65.620	-54.298	-57.820	37.900	7.800	51.300
K(HF2)(a)	78.10305	-946.527	-926.380	-931.233	76.940	15.294	104.264
KI(cr)	166.00277	-342.000	-328.314	-329.300	52.800	12.700	106.050
KNO2(II)	85.10384	-388.840	-368.737	-365.900	107.400	22.940	152.100
KNO3(a)	101.10324	-512.750	-488.307	-494.000	95.060	18.750	132.900
KOH(a)	56.10564	-436.000	-420.338	-423.400	68.930	12.600	81.250
KOH(a)	56.10564	-436.000	-420.338	-423.400	68.930	12.600	81.250
KO2(b)	71.09710	-300.420	-284.652	-283.600	77.530	16.820	125.400
K2CO3(a)	138.20550	-1174.165	-1145.915	-1151.500	114.430	22.665	155.500
K2O(c)	94.19600	-375.400	-356.884	-361.700	72.000	13.700	96.000
K2O2(cr)	110.19540	-460.000	-437.144	-443.000	91.000	17.000	117.000
K2S(cr)	110.26260	(a)	(a)	-376.560	74.684	(a)	115.060
K2SO4(II)	174.26020	-1463.135	-1427.187	-1437.700	131.460	25.435	175.560
K2SiO3(cr)	154.28030	-1564.860	-1534.446	-1543.000	117.570	21.860	146.000
K2Si2O5(a)	214.36460	-2533.820	-2491.509	-2505.000	160.950	28.820	190.580
K3ALF6(II)	258.26686	-3389.600	-3337.321	-3347.000	223.000	42.600	285.000
Li(cr)	6.94100	-4.632	-4.632	0.000	24.860	4.632	29.120
LiALO2(cr)	65.92134	-1198.369	-1180.517	-1188.674	67.777	9.694	53.313

Appendix B (*continued*)

TABLE B2 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
LiBO2(cr)	49.75080	-1031.780	-1017.254	-1022.900	59.800	8.880	51.270
LiBr(cr)	86.84500	-361.636	-344.744	-351.160	49.830	10.476	74.010
LiCL(cr)	42.39370	-417.840	-408.617	-408.540	47.990	9.300	59.270
LiF(cr)	25.93940	-624.773	-615.728	-618.300	41.800	6.473	35.660
LiH(cr)	7.94894	-94.533	-85.667	-90.650	28.950	3.883	20.600
LiI(cr)	133.84547	-284.560	-273.330	-273.200	51.040	11.360	86.710
LiNO2(II)	52.94654	-380.400	-362.753	-368.300	63.000	12.100	88.000
LiNO3(cr)	68.94594	-495.500	-473.513	-482.700	89.000	12.800	104.000
LiOH(cr)	23.94834	-494.914	-481.708	-487.500	49.579	7.414	42.810
Li2CO3(cr)	73.89090	-1229.280	-1205.942	-1214.100	98.320	15.180	90.120
Li2O(cr)	29.88140	-605.131	-591.527	-597.880	54.100	7.251	37.610
Li2O2(cr)	45.88080	-643.000	-625.056	-632.500	75.000	10.500	58.000
Li2SO4(a)	109.94560	-1454.631	-1423.595	-1436.000	117.570	18.631	113.970
Li3ALF6(IV)	161.79496	-3421.750	-3376.839	-3389.600	202.530	32.150	187.900
Li3N(cr)	34.82974	-175.770	-157.539	-164.557	75.266	11.213	62.593
Mg(cr)	24.30500	-4.979	-4.979	0.000	24.775	4.979	32.535
MgAL2O4(cr)	142.26568	-2363.590	-2332.170	-2299.110	116.198	64.480	88.692
MgBr2(cr)	184.11300	-541.500	-512.001	-526.000	73.219	15.500	117.000
MgCO3(cr)	84.31390	-1107.630	-1088.578	-1096.000	76.108	11.631	65.090
MgCL2(cr)	95.21040	-658.070	-643.910	-644.300	71.384	13.770	89.620
MgF2(cr)	62.30181	-1134.120	-1120.316	-1124.200	61.587	9.920	57.200
MgH2(b)	26.32088	-81.010	-67.563	-75.700	35.350	5.310	31.100
MgI2(cr)	278.11394	-387.000	-368.825	-370.000	74.475	17.000	134.000
MgO(cr)	40.30440	-606.760	-597.441	-601.600	37.237	5.160	26.950
Mg(OH)2(cr)	58.31968	-935.760	-913.633	-924.350	77.111	11.410	63.180
MgS(cr)	56.37100	-356.330	-346.939	-348.000	45.560	8.330	50.330
MgSO4(II)	120.36860	-1304.200	-1277.449	-1288.800	96.399	15.400	91.600
MgSiO3(I)	100.38870	-1561.029	-1539.813	-1548.917	81.927	12.113	67.768
MgTiO3(cr)	120.17020	-1586.113	-1563.289	-1572.556	91.881	13.556	74.559
MgTi2O5(cr)	200.03600	-2530.658	-2494.330	-2508.219	146.858	22.439	135.603
Mg2SiO4(cr)	140.69310	-2194.358	-2163.822	-2177.078	118.688	17.280	95.140
Mg2TiO4(cr)	160.47460	-2183.191	-2151.048	-2164.354	128.574	18.836	115.102
Mg3N2(cr)	100.92848	-471.800	-448.193	-461.300	92.049	10.500	85.000
Mn(a)	54.93805	-4.994	-4.994	0.000	26.299	4.994	32.010
Mo(cr)	95.94000	-4.585	-4.585	0.000	23.933	4.585	28.605
MoO2(cr)	127.93880	-597.628	-584.363	-589.300	55.910	8.328	46.510
MoO3(cr)	143.93820	-757.190	-739.585	-744.600	75.070	12.590	77.660
NH4CL(II)	53.49120	-337.251	-311.389	-314.553	86.441	22.698	94.860
NH4F(cr)	37.03690	-478.668	-452.984	-467.560	65.269	11.108	71.970
Na(cr)	22.98977	-6.460	-6.460	0.000	28.230	6.460	51.300
NaALO2(a)	81.97011	-1156.984	-1137.304	-1133.190	73.638	23.794	70.400
NaBO2(cr)	65.79957	-988.132	-971.778	-976.500	65.940	11.632	73.530
NaBr(cr)	102.89377	-372.750	-354.030	-361.160	51.380	11.590	86.930
NaCN(II)	49.00721	-110.131	-98.283	-90.709	69.036	19.422	118.457
NaCL(cr)	58.44247	-421.860	-410.809	-411.260	50.500	10.600	72.150
NaF(cr)	41.98817	-585.082	-574.209	-576.600	46.820	8.482	51.160
NaH(cr)	23.99771	-62.639	-51.945	-56.380	36.400	6.259	40.000
NaI(cr)	149.89424	-301.890	-288.832	-289.630	52.090	12.260	98.560
NaNO2(I)	68.99531	-371.100	-351.625	-354.600	69.000	16.500	106.000
NaNO3(a)	84.99471	-484.930	-461.115	-467.700	93.050	17.230	116.400
NaOH(a)	39.99711	-436.290	-421.256	-425.800	59.530	10.490	64.430
NaO2(cr)	54.98857	-279.300	-264.160	-261.000	72.130	18.300	115.900
Na2CO3(a)	105.98844	-1149.940	-1122.946	-1129.190	112.300	20.750	135.000
Na2O(c)	61.97894	-426.970	-409.710	-414.570	69.120	12.400	75.040
Na2O2(b)	77.97834	-527.694	-506.094	-512.000	89.330	15.694	94.770

Appendix B (*continued*)

TABLE B2 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
Na2S(cr)	78.04554	(a)	(a)	-366.100	82.801	(a)	96.232
Na2SO3(cr)	126.04374	(a)	(a)	-1100.802	120.247	(a)	145.938
Na2SO4(V)	142.04314	-1411.104	-1376.412	-1387.900	128.040	23.204	149.580
Na3ALF6(a)	209.94127	-3360.470	-3310.075	-3322.400	215.900	38.070	238.200
Na5AL3F14(cr)	461.87111	-7635.830	-7528.134	-7555.000	454.000	80.830	515.200
Nb(cr)	92.90638	-5.241	-5.241	0.000	24.694	5.241	36.464
NbO(cr)	108.90578	-413.200	-403.619	-406.000	41.000	7.200	46.000
NbOCL3(cr)	215.26388	(a)	(a)	-879.500	119.820	(a)	142.000
NbO2(II)	124.90518	-804.267	-790.346	-795.000	57.660	9.267	54.290
Nb2O5(cr)	265.80976	-1919.240	-1887.058	-1897.000	131.950	22.240	137.100
Ni(cr)	58.69340	-4.786	-4.786	0.000	25.987	4.786	29.870
NiS(b)	90.75940	-96.329	-87.131	-87.864	47.112	8.465	52.992
NiS2(cr)	122.82540	(a)	(a)	-131.378	70.626	(a)	71.965
Ni3S2(a)	240.21220	-239.142	-215.960	-217.986	117.654	21.156	133.888
Ni3S4(cr)	304.34420	(a)	(a)	-301.115	164.808	(a)	186.481
P(cr)	30.97376	-5.360	-5.360	0.000	23.824	5.360	41.090
P4O10(cr)	283.88904	-3044.320	-2979.479	-3010.100	215.569	34.220	231.000
Pb(cr)	207.20000	-6.870	-6.870	0.000	26.650	6.870	64.800
PbBr2(cr)	367.00800	-295.930	-264.540	-276.700	79.580	19.230	161.100
PbCL2(cr)	278.10540	-376.550	-360.499	-359.400	76.985	17.150	136.000
PbF2(II)	245.19681	-691.000	-675.305	-676.000	72.259	15.000	106.000
PbI2(cr)	461.00894	-195.500	-175.434	-176.000	77.570	19.500	174.850
PbO(II-r)	223.19940	-227.825	-216.615	-218.600	46.414	9.225	67.840
PbO2(cr)	239.19880	-286.962	-271.412	-276.000	60.997	10.962	71.920
PbS(cr)	239.26600	-110.985	-99.703	-99.475	49.499	11.510	91.200
Pb2O3(cr)	462.39820	-512.580	-485.820	-491.700	107.701	20.880	151.900
Pb3O4(cr)	685.59760	-749.830	-711.860	-720.000	146.705	29.830	211.300
Rb(cr)	85.46780	-7.489	-7.489	0.000	31.060	7.489	76.780
RbBO2(b)	128.27760	-988.310	-970.927	-975.000	73.390	13.310	94.320
RbBr(cr)	165.37180	-407.830	-388.081	-394.770	52.760	13.060	110.100
RbCL(cr)	120.92050	-447.380	-435.300	-435.220	52.260	12.160	95.230
RbF(cr)	104.46620	-570.600	-558.698	-559.700	50.630	10.900	77.700
RbH(cr)	86.47574	-61.400	-49.677	-52.300	39.300	9.100	63.700
RbI(cr)	212.37227	-346.940	-332.853	-333.600	52.590	13.340	118.800
RbNO2(I)	131.47334	-390.400	-369.896	-367.000	84.000	23.400	162.000
RbNO3(IV)	147.47274	-514.340	-489.496	-494.700	99.000	19.640	144.900
RbOH(b)	102.47514	-432.300	-416.237	-418.800	69.000	13.500	94.000
RbO2(b)	117.46660	-295.860	-279.691	-279.100	77.570	16.760	130.100
Rb2CO3(a)	230.94450	-1157.080	-1128.028	-1132.600	117.600	24.480	181.330
Rb2O(c)	186.93500	-353.600	-334.282	-338.000	74.000	15.600	125.000
Rb2O2(b)	202.93440	-429.700	-406.042	-410.000	93.000	19.700	160.000
Rb2SO4(a)	266.99920	-1462.914	-1426.164	-1435.900	134.055	27.014	197.500
S(a)	32.06600	-4.412	-4.412	0.000	22.690	4.412	32.070
SCL2(L)	102.97140	(a)	(a)	-49.790	91.002	(a)	183.678
S2CL2(L)	135.03740	(a)	(a)	-58.158	124.290	(a)	223.844
Sc(a)	44.95591	-5.207	-5.207	0.000	25.510	5.207	34.770
Sc2O3(cr)	137.91002	-1922.530	-1899.096	-1908.600	94.220	13.930	76.800
Si(cr)	28.08550	-3.217	-3.217	0.000	19.789	3.217	18.810
SiC(b)	40.09620	-76.272	-72.001	-73.000	26.860	3.272	16.610
SiO2(a-qz)	60.08430	-917.616	-905.718	-910.700	44.602	6.916	41.460
SiS(cr)	60.15150	-177.738	-170.108	-168.737	45.000	9.000	63.000
SiS2(cr)	92.21750	-298.180	-286.139	-287.000	61.630	11.180	76.860
Si2N2O(cr)	100.18388	(a)	(a)	-947.700	65.560	(a)	45.350
Si3N4(cr)	140.28346	-799.913	-772.921	-787.800	93.010	12.113	66.065
Sn(cr)	118.71000	-6.323	-6.323	0.000	27.112	6.323	51.180

Appendix B (*continued*)

TABLE B2 (*continued*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	T = 298.15 K: $\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
SnBr2(cr)	278.51800	-272.270	-241.427	-253.600	78.970	18.670	153.000
SnBr4(cr)	438.32600	-419.260	-363.897	-388.000	133.300	31.260	260.000
SnCL2(cr)	189.61540	-350.330	-334.826	-333.000	78.051	17.330	134.100
SnCL4(L)	260.52080	-555.740	-531.055	-517.000	157.400	38.740	265.000
SnF2(cr)	156.70681	-691.200	-676.052	-677.000	72.395	14.200	96.200
SnI2(cr)	372.51894	-171.950	-152.431	-153.000	78.310	18.950	168.500
SnI4(cr)	626.32788	-239.100	-206.385	-207.500	131.550	31.600	282.700
SnO(cr)	134.70940	-289.446	-278.783	-280.710	47.783	8.736	57.170
SnO2(cr)	150.70880	-586.014	-571.011	-577.630	53.219	8.384	49.010
SnS(cr)	150.77600	-120.192	-109.457	-109.662	49.245	10.530	77.000
SnS2(cr)	182.84200	-155.147	-140.000	-141.837	70.123	13.310	87.400
Sr(a)	87.62000	-6.558	-6.558	0.000	26.830	6.558	54.999
SrBr2(a)	247.42800	-740.060	-708.982	-722.000	76.527	18.060	143.440
SrCO3(a)	147.62890	-1241.120	-1220.489	-1226.000	82.424	15.121	97.200
SrCL2(a)	158.52540	-849.230	-833.491	-833.000	75.605	16.230	114.850
SrF2(a)	125.61681	-1242.075	-1226.692	-1229.000	70.000	13.075	82.130
SrH2(a)	89.63588	-188.000	-172.974	-180.000	44.000	8.000	52.000
SrI2(cr)	341.42894	-586.920	-567.166	-568.000	77.404	18.920	159.100
SrO(cr)	103.61940	-599.680	-588.782	-591.000	45.250	8.680	55.580
Sr(OH)2(b)	121.63468	-979.572	-955.866	-964.300	89.220	15.272	94.990
SrS(cr)	119.68600	-490.040	-479.070	-480.000	48.700	10.041	68.200
SrS04(a)	183.68360	-1475.400	-1447.070	-1457.000	102.000	18.400	121.000
Ta(cr)	180.94790	-5.681	-5.681	0.000	25.295	5.681	41.471
TaC(cr)	192.95860	-150.611	-143.877	-144.097	36.790	6.514	42.371
Ta2O5(II)	441.89280	-2071.950	-2038.888	-2049.000	134.935	22.950	141.900
Th(a)	232.03810	-6.350	-6.350	0.000	26.230	6.350	51.830
Ti(a)	47.86700	-4.824	-4.824	0.000	25.060	4.824	30.720
TiB(cr)	58.67800	(a)	(a)	-160.247	29.673	(a)	34.727
TiB2(cr)	69.48900	-285.068	-277.816	-279.491	44.279	5.577	28.485
TiC(cr)	59.87770	-188.703	-182.825	-184.096	33.807	4.607	24.230
TiCL2(cr)	118.77240	-528.771	-514.766	-515.470	69.831	13.301	87.345
TiCL3(cr)	154.22510	-742.660	-724.064	-721.740	97.161	20.920	139.750
TiCL4(L)	189.67780	-831.128	-807.942	-804.165	145.205	26.963	252.379
TiN(cr)	61.87374	-343.136	-333.977	-337.649	37.079	5.487	30.234
TiO(a)	63.86640	-548.175	-539.011	-542.000	39.905	6.175	34.790
TiO2(cr)	79.86580	-952.680	-939.176	-944.000	55.080	8.680	50.620
Ti2O3(I)	143.73220	-1534.090	-1511.422	-1520.000	95.810	14.090	77.290
Ti3O5(a)	223.59800	-2479.630	-2443.458	-2457.000	150.830	22.630	126.200
Ti4O7(cr)	303.46380	-3438.630	-3388.954	-3403.000	216.810	35.630	201.480
U(a)	238.02890	-6.364	-6.364	0.000	27.665	6.364	50.200
UF3(cr)	295.02411	-1527.080	-1507.478	-1508.700	95.100	18.380	123.400
UF4(cr)	314.02251	-1943.050	-1919.036	-1920.500	116.020	22.550	151.670
UF5(b)	333.02092	-2109.150	-2080.723	-2083.000	132.000	26.150	179.500
UF6(cr)	352.01932	-2229.265	-2196.426	-2197.700	166.750	31.565	227.800
UO2(cr)	270.02770	-1096.280	-1081.236	-1085.000	63.600	11.280	77.030
UO2F2(cr)	308.02451	-1673.300	-1649.431	-1653.600	103.200	19.700	135.500
UO3(c)	286.02710	-1238.385	-1219.001	-1223.800	81.670	14.585	96.110
U3O8(II)	842.08190	-3617.540	-3563.728	-3574.800	238.338	42.740	282.549
U4O9(III)	1096.11020	-4562.750	-4498.234	-4512.000	293.340	50.750	334.130
V(cr)	50.94150	-4.640	-4.640	0.000	24.896	4.640	28.936
VCL2(cr)	121.84690	(a)	(a)	-451.872	71.868	(a)	97.069
VCL3(cr)	157.29960	(a)	(a)	-581.116	93.174	(a)	130.959
VN(cr)	64.94824	-223.376	-214.401	-217.150	37.982	6.226	37.263
VO(cr)	66.94090	-436.780	-427.800	-430.800	38.420	5.980	33.510
V2O3(cr)	149.88120	-1233.930	-1211.630	-1216.800	100.960	17.130	94.490

Appendix B (*continued*)

TABLE B2 (*concluded*)

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	$T = 298.15$ K: $\Delta_f H^o(T)$ kJ/mol	$T = 298.15$ K: $C_p^o(T)$ J/K-mol	$T = 298.15$ K: $H^o(T) - H^o(0)$ kJ/mol	$T = 298.15$ K: $S^o(T)$ J/K-mol
V2O4(II)	165.88060	-1449.320	-1422.680	-1432.600	112.130	16.720	93.180
V2O5(cr)	181.88000	-1572.210	-1541.230	-1551.000	127.770	21.210	130.500
W(cr)	183.84000	-4.973	-4.973	0.000	24.295	4.973	32.660
WC(cr)	195.85070	(a)	(a)	-40.540	35.378	(a)	32.384
WCL6(I)	396.55620	(a)	(a)	-593.710	175.418	(a)	238.488
WOCL4(cr)	341.65020	(a)	(a)	-671.114	146.248	(a)	172.799
WO2(cr)	215.83880	-596.811	-583.158	-588.100	55.780	8.711	50.640
WO2CL2(cr)	286.74420	(a)	(a)	-780.316	104.408	(a)	200.832
WO3(III)	231.83820	-854.580	-836.587	-841.300	79.705	13.280	81.640
Zn(cr)	65.39000	-5.657	-5.657	0.000	25.390	5.657	41.630
ZnSO4(a)	161.45360	-997.382	-969.953	-980.144	99.035	17.238	110.541
Zr(a)	91.22400	-5.497	-5.497	0.000	25.202	5.497	38.869
ZrC(cr)	103.23470	-202.510	-195.959	-196.648	37.899	5.862	33.321
ZrN(cr)	105.23074	-377.828	-367.996	-371.238	40.443	6.590	38.861
ZrO2(III)	123.22280	-1109.051	-1094.874	-1100.300	55.920	8.751	50.390
CH3OH(L)	32.04186	-257.905	-235.575	-238.910	81.080	18.995	127.270
C2H5OH(L)	46.06844	-301.592	-269.741	-277.510	112.250	24.082	160.100
C6H6(L)	78.11184	18.970	50.695	49.080	135.950	30.110	173.440
C6H5NH2(L)	93.12652	-2.520	37.774	31.500	191.920	34.020	191.060
C6H14(L),n-hexa	86.17536	-245.580	-179.982	-198.660	195.480	46.920	296.090
C7H8(L)	92.13842	-21.290	19.957	12.180	157.290	33.470	221.030
C7H16(L),n-hept	100.20194	-276.990	-201.871	-224.350	224.980	52.640	328.560
C8H18(L),n-octa	114.22852	-311.750	-227.109	-250.260	254.150	61.490	361.070
C8H18(L),isooct	114.22852	-309.350	-224.709	-259.160	239.000	50.190	328.110
H2O2(L)	34.01468	-210.729	-193.581	-187.780	89.330	22.949	109.602
Jet-A(L)	167.31102	(a)	(a)	-303.403	350.332	(a)	448.106
NH4CLO4(I)	117.48880	-321.005	-277.783	-295.767	128.072	25.238	184.180
NH4NO3(IV)	80.04344	-389.262	-350.636	-365.600	139.080	23.662	150.810
N2H4(L)	32.04524	(a)	(a)	50.380	98.840	(a)	121.544

[a]No data available for 0 K.

Appendix B (*continued*)

TABLE B3.—ASSIGNED ENTHALPIES FOR SPECIES THAT ARE USED IN CEA AS REACTANTS ONLY

Species name	Phase	Stoichiometry									Molecular weight	$H^o(T)$	T K
Air	gas	[a]N	1.56	O	0.42	Ar	0.01	C	0.00		28.96518	-0.126	298.15
B2H6(L)	liq	B	2.00	H	6.00		0.00		0.00		27.66964	16.445	180.59
B5H9(L)	liq	B	5.00	H	9.00		0.00		0.00		63.12646	42.840	298.15
(CH2)x(cr)	sol	C	1.00	H	2.00		0.00		0.00		14.02658	-25.600	298.15
CH3NO2(L)	liq	C	1.00	H	3.00	N	1.00	O	2.00		61.04006	-113.100	298.15
CH4(L)	liq	C	1.00	H	4.00		0.00		0.00		16.04246	-89.233	111.64
CH3OH(L)	liq	C	1.00	H	4.00	O	1.00		0.00		32.04186	-238.910	298.15
CH6N2(L)	liq	C	1.00	H	6.00	N	2.00		0.00		46.07182	54.200	298.15
C2H2(L),acetyle	liq	C	2.00	H	2.00		0.00		0.00		26.03728	207.599	192.35
CH3CN(L)	liq	C	2.00	H	3.00	N	1.00		0.00		41.05196	31.380	298.15
C2H4(L)	liq	C	2.00	H	4.00		0.00		0.00		28.05316	33.945	169.42
C2H4O(L),ethyle	liq	C	2.00	H	4.00	O	1.00		0.00		44.05256	-78.841	283.65
C2H6(L)	liq	C	2.00	H	6.00		0.00		0.00		30.06904	-103.819	184.56
C2H5OH(L)	liq	C	2.00	H	6.00	O	1.00		0.00		46.06844	-277.510	298.15
C2H8N2(L),UDMH	liq	C	2.00	H	8.00	N	2.00		0.00		60.09840	48.900	298.15
C2N2(L)	liq	C	2.00	N	2.00		0.00		0.00		52.03488	283.209	252.05
C3H6(L),propyle	liq	C	3.00	H	6.00		0.00		0.00		42.07974	-2.704	225.46
C3H7NO3(L)	liq	C	3.00	H	7.00	N	1.00	O	3.00		105.09262	-214.500	298.15
C3H8(L)	liq	C	3.00	H	8.00		0.00		0.00		44.09562	-128.228	231.08
C4H8(L),1-buten	liq	C	4.00	H	8.00		0.00		0.00		56.10632	-25.173	266.92
C4H10(L),n-buta	liq	C	4.00	H	10.00		0.00		0.00		58.12220	-150.664	272.64
C4H10(L),isobut	liq	C	4.00	H	10.00		0.00		0.00		58.12220	-159.664	261.36
C5H12(L),n-pent	liq	C	5.00	H	12.00		0.00		0.00		72.14878	-173.490	298.15
C6H6(L)	liq	C	6.00	H	6.00		0.00		0.00		78.11184	49.080	298.15
C6H5NH2(L)	liq	C	6.00	H	7.00	N	1.00		0.00		93.12652	31.500	298.15
C6H14(L),n-hexa	liq	C	6.00	H	14.00		0.00		0.00		86.17536	-198.660	298.15
C7H8(L)	liq	C	7.00	H	8.00		0.00		0.00		92.13842	12.180	298.15
C7H16(L),n-hept	liq	C	7.00	H	16.00		0.00		0.00		100.20194	-224.350	298.15
C8H18(L),n-octa	liq	C	8.00	H	18.00		0.00		0.00		114.22852	-250.260	298.15
C8H18(L),isooct	liq	C	8.00	H	18.00		0.00		0.00		114.22852	-259.160	298.15
CLF3(L)	liq	CL	1.00	F	3.00		0.00		0.00		92.44791	-193.386	284.89
CLO3F	gas	CL	1.00	O	3.00	F	1.00		0.00		102.44930	-23.800	298.15
CLO3F(L)	liq	CL	1.00	O	3.00	F	1.00		0.00		102.44930	-47.436	226.40
CL2(L)	liq	CL	2.00		0.00		0.00		0.00		70.90540	-22.550	239.12
F2(L)	liq	F	2.00		0.00		0.00		0.00		37.99681	-13.091	85.02
F2O(L)	liq	F	2.00	O	1.00		0.00		0.00		53.99621	6.672	128.40
HNO3(L)	liq	H	1.00	N	1.00	O	3.00		0.00		63.01288	-173.013	298.15
H2(L)	liq	H	2.00		0.00		0.00		0.00		2.01588	-9.012	20.27
H2O2(L)	liq	H	2.00	O	2.00		0.00		0.00		34.01468	-187.780	298.15
IRFNA	liq	H	1.57	N	1.63	O	4.70	F	0.02		100.00000	-270.496	298.15
JP-4	liq	C	1.00	H	1.94		0.00		0.00		13.96842	-22.723	298.15
JP-5	liq	C	1.00	H	1.92		0.00		0.00		13.94443	-22.183	298.15
JP-10(L)	liq	C	10.00	H	16.00		0.00		0.00		136.23404	-122.800	298.15
JP-10(g)	gas	C	10.00	H	16.00		0.00		0.00		136.23404	-86.856	298.15
Jet-A(L)	liq	C	12.00	H	23.00		0.00		0.00		167.31102	-303.403	298.15
Jet-A(g)	gas	C	12.00	H	23.00		0.00		0.00		167.31102	-249.657	298.15
LiCLO4(cr)	sol	LI	1.00	CL	1.00	O	4.00		0.00		106.39130	-380.700	298.15
NF3(L)	liq	N	1.00	F	3.00		0.00		0.00		71.00195	-150.387	144.09
NH3(L)	liq	N	1.00	H	3.00		0.00		0.00		17.03056	-71.555	239.72
NH4CLO4(I)	liq	N	1.00	H	4.00	CL	1.00	O	4.00		117.48880	-295.767	298.15

[a]Stoichiometry for air: N, 1.56168; O, 0.419590; Ar, 0.009365; C, 0.000319.

Appendix B (*concluded*)

TABLE B3 (*concluded*)

Species name	Phase	Stoichiometry							Molecular weight	$H°(T)$	T K
NH4NO3(I)	liq	N	2.00	H	4.00	O	3.00	0.00	80.04344	-365.600	298.15
N2(L)	liq	N	2.00		0.00		0.00	0.00	28.01348	-12.107	77.35
N2H4(L)	liq	N	2.00	H	4.00		0.00	0.00	32.04524	50.380	298.15
N2O4(L)	liq	N	2.00	O	4.00		0.00	0.00	92.01108	-17.549	298.15
O2(L)	liq	O	2.00		0.00		0.00	0.00	31.99880	-12.979	90.17
O3(L)	liq	O	3.00		0.00		0.00	0.00	47.99820	122.527	161.85
RP-1	liq	C	1.00	H	1.95		0.00	0.00	13.97820	-24.717	298.15

Appendix C
Format for Thermodynamic Data Coefficients

This appendix explains the format for data contained in the file thermo.inp (app. D). Equations (1) to (3) are repeated here for convenience:

$$C_p^o(T)/R = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4 \quad (1)$$

$$H^o(T)/RT = -a_1T^{-2} + a_2 lnT/T + a_3 + a_4T/2 + a_5T^2/3 + a_6T^3/4 + a_7T^4/5 + b_1/T \quad (2)$$

$$S^o(T)/R = -a_1T^{-2}/2 - a_2T^{-1} + a_3 lnT + a_4T + a_5T^2/2 + a_6T^3/3 + a_7T^4/4 + b_2 \quad (3)$$

TABLE C1.—FORTRAN FORMAT USED FOR DATA IN APPENDIX D

Record	Contents	FORTRAN format	Columns
1	Species name or formula	A16	1 to 16
	Comments and data sources	A62	19 to 80
2	Number of T intervals	I2	1 to 2
	Reference date code	A6	4 to 9
	Chemical formula—symbols (all capitals) and numbers	5(A2, F6.2)	11 to 50
	Zero for gas; nonzero for condensed[a]	I2	51 to 52
	Molecular weight	F13.7	53 to 65
	Heat of formation at 298.15 K, J/mol	F15.5	66 to 80
3	Temperature range	2F11.3	1 to 22
	Number of coefficients for $C_p^o(T)/R$ (always seven)	I1	23
	T exponents in empirical equation for $C_p^o(T)/R$ [always −2, −1, 0, 1, 2, 3, 4; see eq. (1)]	8F5.1	24 to 63
	$H^o(298.15) - H^o(0)$ J/mol, if available	F15.3	66 to 80
4	First five coefficients for $C_p^o(T)/R$, eq. (1)	5D16.9	1 to 80
5	Last two coefficients for $C_p^o(T)/R$, eq. (1)	2D16.9	1 to 32
	Integration constants b_1 and b_2, eqs. (2) and (3)	2D16.9	49 to 80
-	Repeat 3, 4, and 5 for each interval	---------	---------

[a] Condensed phases are numbered in increasing order by temperature.

For example, the following data are for condensed titanium nitride:

```
    12345678901234567890123456789012345678901234567890123456789012345678901234567890
             10        20        30        40        50        60        70        80

1   TiN(cr)           Chase,1998 pp1612-4.                                          1
2    2 j 6/68 TI  1.00N   1.00    0.00    0.00    0.00 1     61.87374    -337648.800  2
3       200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5487.000  3
4   -5.479117220D+05 9.328691110D+03-6.386263890D+01 2.429925456D-01-4.304234520D-04  4
5    3.792645100D-07-1.317412256D-10                -8.424256140D+04 3.392988560D+02  5
6       800.000   3220.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5487.000  6
7   -3.656247060D+05 1.265730431D+03 3.831711190D+00 1.632900455D-03-1.062786626D-07  7
8    1.310931390D-11-5.770548410D-16                -5.027654400D+04-1.652632899D+01  8
9   TiN(L)            Chase,1998 pp1612-4.                                          9
10   1 j 6/68 TI  1.00N   1.00    0.00    0.00    0.00 2     61.87374    -337648.800 10
11     3220.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5487.000 11
12   0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00 12
13   0.000000000D+00 0.000000000D+00                -3.626039860D+04-3.958296649D+01 13

    12345678901234567890123456789012345678901234567890123456789012345678901234567890
             10        20        30        40        50        60        70        80
```

Appendix C (*concluded*)

There are two sets of data: one for the crystal and one for the liquid. We focus first on the crystalline phase (records 1 to 8): record 1 lists the name as TiN(cr) and tells us that the data for this phase originated from Chase (1998), pp. 1612–1614. Record 2 gives the following information:

TABLE C2.—EXPLANATION OF SECOND RECORD FOR TiN(cr) DATA

Columns	Contents	Explanation
2	2	Number of intervals covered by the data
4 to 9	j 6/68	Internal NASA reference code (see app. D)
11 to 26	Tl 1.00N 1.00	Molecular formula [unused places (11 to 50) filled with blanks and zeros]
52	1	(First) condensed phase
58 to 65	61.87374	Molecular weight
70 to 80	-337648.800	$\Delta_f H°(298.15)$ in J/mol

Records 3 to 5 cover the temperature interval 200 to 800 K. The single digit "7" after the temperature range says that $C_p^\circ(T)/R$ is described by seven coefficients in each interval. The next eight 5-place fields on record 3 list the temperature exponents in the empirical equation for $C_p^\circ(T)/R$ used in this temperature interval. The last entry on record 3 contains a value of 5487.00 J/mol for $H°(298.15) - H°(0)$. This field will contain the number 0.0000 if $H°(298.15) - H°(0)$ is not available. Records 4 to 5 contain the coefficients a_1 through a_7, b_1, and b_2 for TiN(cr) for the temperature range 200 to 800 K; records 7 to 8 contain these coefficients for the temperature range 800 to 3220 K. Both intervals use equation (1) to describe $C_p^\circ(T)/R$.

Immediately following the TiN(cr) data block are data for the liquid. The temperature range 3220 K (melting point) to 6000 K is covered by one set of coefficients, again with seven terms for $C_p^\circ(T)/R$ and again in the form of equation (1). The zero values listed for all constants except a_3 indicate that the heat capacity is a constant, and in accordance with equation (1), $C_p^\circ(T)/R = 7.548249987$.

Appendix D
Listing of NASA Glenn Thermodynamic Data Coefficients

The remainder of this appendix is a listing of the data file "thermo.inp," which is the subject of this report. The initial lines that start with an exclamation point are comments. See the text and Appendix C for a further explanation of these data.

```
!          SIX-CHARACTER REFERENCE-DATE CODES
!
!  Letters          Reference                        Numbers
!
!    j       NIST-JANAF Thermochemical              Month/year of table
!            Tables. Chase,1998
!
!    tpis    Thermodynamic Properties of            Year of volume
!            Individual Substances. Gurvich,
!            1978,1979,1982,1989,1991,1996
!
!    n       TRC Thermodynamic Tables, NIST         Month/year of table
!
!    bar     Barin: Thermochemical Data of          Year of volume
!            Pure Substances. Barin,1989
!
!    coda    CODATA Key Values for                  Year of volume
!            Thermodynamics. Cox,1989
!
!    srd     Standard Reference Data                Year of J. Phys. Chem. Ref.
!                                                   Data journal
!
!
!                    ORDER OF SPECIES

1)     Gaseous products/reactants, pages 45-210
2)     Condensed products/reactants, pages 210-276
3)     Gaseous/condensed reactants only, pages 276-280


thermo
    200.00   1000.00   6000.00  20000.      3/19/02
e-                Ref-Species. Chase,1998 3/82.
 3 g12/98 E   1.00     0.00     0.00     0.00     0.00 0.000548579903          0.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02-1.172081224D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02-1.172081224D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02-1.172081224D+01
Ag               Hf:Cox,1989. Moore,1971. Gordon,1999.
 3 g10/97 AG  1.00     0.00     0.00     0.00     0.00 0  107.8682000     284900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.352002370D+04 6.562819350D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-3.309926370D+05 9.820086420D+02 1.381179917D+00 6.170899990D-04-1.688114600D-07
 2.008826848D-11-5.627285655D-16                 2.726719171D+04 1.456862733D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-3.717441500D+08 2.758069172D+05-7.385982610D+01 9.606158720D-03-5.393935740D-07
 1.358856730D-11-1.272610104D-16                -2.107724971D+06 6.628374570D+02
```

Appendix D (*continued*)

```
Ag+                Moore,1971. Gordon,1999.
 3 g10/97 AG  1.00E  -1.00    0.00    0.00    0.00 0  107.8676514    1022093.730
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.530
 3.691132750D+06-4.316983000D+04 2.028445385D+02-4.658413740D-01 5.586200510D-04
-3.154880975D-07 6.578702060D-11                 3.371574470D+05-1.142924427D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.530
-5.327432350D+07 1.310710631D+05-1.098820208D+02 4.826002760D-02-1.093661557D-05
 1.263835910D-09-5.852542535D-14                -7.439122510D+05 8.446266190D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.530
-2.119469170D+08 1.159621936D+05-2.220792532D+01 2.938747589D-03-1.822389545D-07
 5.823925360D-12-7.455184012D-17                -8.068014150D+05 2.271702823D+02
Ag-                Hotop,1985. Gordon,1999.
 3 g10/97 AG  1.00E   1.00    0.00    0.00    0.00 0  107.8687486     153078.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.766565919D+04 5.869679800D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.766565919D+04 5.869679800D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.766565919D+04 5.869679800D+00
AL                 Hf:Cox,1989. Kaufman,1991b. Gordon,1999.
 3 g12/97 AL  1.00    0.00    0.00    0.00    0.00 0   26.9815380     330000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6918.671
 5.006608890D+03 1.861304407D+01 2.412531111D+00 1.987604647D-04-2.432362152D-07
 1.538281506D-10-3.944375734D-14                 3.887412680D+04 6.086585765D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6918.671
-2.920820938D+04 1.167751876D+02 2.356906505D+00 7.737231520D-05-1.529455262D-08
-9.971670260D-13 5.053278264D-16                 3.823288650D+04 6.600920155D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6918.671
-5.040682320D+08 3.802322650D+05-1.082347159D+02 1.549444292D-02-1.070103856D-06
 3.592110900D-11-4.696039394D-16                -2.901050501D+06 9.491883160D+02
AL+                Kaufman,1991b. Moore,1971. Gordon,1999.
 3 g 1/98 AL  1.00E  -1.00    0.00    0.00    0.00 0   26.9809894     913015.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.090644788D+05 3.791005780D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-4.181183250D+03-9.948557270D+00 2.548615878D+00-5.878760040D-05 3.132291294D-08
-7.748894630D-12 7.274447690D-16                 1.091011485D+05 3.488667290D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-9.080958540D+08 5.509673040D+05-1.279244177D+02 1.510503026D-02-8.932051950D-07
 2.719381070D-11-3.367986284D-16                -4.268693020D+06 1.141245444D+03
AL-                Chase,1998 p65 6/83. EA:Hotop,1985. Gordon,1999.
 3 g 3/97 AL  1.00E   1.00    0.00    0.00    0.00 0   26.9820866     281090.113
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6756.213
 2.910801723D+04-3.836983750D+02 4.655142800D+00-6.045821840D-03 8.577259640D-06
-5.476260000D-09 1.322714061D-12                 3.490616980D+04-5.957097700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6756.213
 6.339814320D+05-2.383438463D+03 5.469971130D+00-1.299840355D-03 2.888305470D-07
-3.253240510D-11 1.472436088D-15                 4.780306540D+04-1.536906816D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6756.213
 5.901212850D+06-2.296000877D+03 3.072774844D+00-6.894714790D-05 4.413313240D-09
-1.445353715D-13 1.905752608D-18                 5.241871250D+04 1.451781383D+00
ALBr               Gurvich,1996a pt1 p184 pt2 p148.
 2 tpis96 AL  1.00BR  1.00    0.00    0.00    0.00 0  106.8855380      14325.015
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9571.115
 8.176158640D+03-2.516942718D+02 5.403296330D+00-1.747212920D-03 2.077304770D-06
-1.261267579D-09 3.166335970D-13                 1.635024429D+03-2.323594886D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9571.115
-6.103395600D+05 2.010066834D+03 1.769617961D+00 1.929888914D-03-6.641047830D-07
 1.172854627D-10-7.178742760D-15                -1.217812867D+04 2.204450764D+01
ALBr2              Gurvich,1996a pt1 p186 pt2 p149.
 2 tpis96 AL  1.00BR  2.00    0.00    0.00    0.00 0  186.7895380    -140662.125
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13397.875
 3.199375870D+04-7.119178970D+02 9.478258110D+00-4.875531670D-03 5.516512990D-06
-3.340053040D-09 8.368476840D-13                -1.540591306D+04-1.742171366D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13397.875
-3.523782900D+05 4.671544170D+02 7.111908190D+00-5.551709200D-04 3.166301130D-07
-5.521028330D-11 3.176725950D-15                -2.265004078D+04-2.695610360D+00
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Appendix D (*continued*)

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ALBr3              Gurvich,1996a pt1 p188 pt2 p151.
 2 tpis96 AL  1.00BR  3.00    0.00    0.00    0.00 0  266.6935380    -410476.664
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17943.336
 4.718948840D+04-1.053853163D+03 1.350747168D+01-6.639869930D-03 7.269276830D-06
-4.278049490D-09 1.045573281D-12                -4.699440330D+04-3.667936780D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17943.336
-8.935527440D+04-2.678035134D+01 1.002063997D+01-8.458764400D-06 1.904243317D-09
-2.215195785D-13 1.038219389D-17                -5.249247640D+04-1.579666403D+01
ALC                Gurvich,1996a pt1 p205 pt2 p165.
 2 tpis96 AL  1.00C   1.00    0.00    0.00    0.00 0   38.9922380     682283.509
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9058.109
 4.139921880D+04-5.858677890D+02 5.962445720D+00-2.006064322D-03 1.665566136D-06
-7.121649210D-10 1.271188744D-13                 8.383436110D+04-8.002165050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9058.109
 1.937001487D+06-6.749117790D+03 1.347525643D+01-5.850802650D-03 1.926461091D-06
-2.585922351D-10 1.222659806D-14                 1.225363649D+05-6.152244872D+01
ALC2               Gurvich,1996a pt1 p206 pt2 p166.
 2 tpis96 AL  1.00C   2.00    0.00    0.00    0.00 0   51.0029380     675615.776
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12262.776
 1.524087465D+04-2.649987059D+02 6.280414900D+00-1.786037647D-04 3.791907740D-06
-3.999450070D-09 1.299752388D-12                 8.092763280D+04-6.247291862D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12262.776
 1.466017895D+05-1.362764489D+03 8.457759150D+00-3.678901680D-04 7.903174500D-08
-8.880023720D-12 4.053633950D-16                 8.705924230D+04-2.127956728D+01
ALCL               Gurvich,1996a pt1 p168 pt2 p131.
 2 tpis96 AL  1.00CL  1.00    0.00    0.00    0.00 0   62.4345380     -51007.443
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9323.112
 2.380881392D+04-4.457159420D+02 5.992853990D+00-2.777300261D-03 3.101582418D-06
-1.815268376D-09 4.414662340D-13                -5.202736030D+03-7.383298016D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9323.112
-8.993461220D+05 2.765942061D+03 1.003500696D+00 2.267806833D-03-7.280541600D-07
 1.182380673D-10-6.660498130D-15                -2.496164448D+04 2.616925480D+01
ALCL+              Chase,1998 p73.
 2 j 6/76 AL  1.00CL  1.00E  -1.00    0.00    0.00 0   62.4339894     861849.307
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9154.435
 3.469955220D+04-5.479900030D+02 6.106011130D+00-2.674711519D-03 2.696426573D-06
-1.463885068D-09 3.358729060D-13                 1.051719510D+05-7.816586372D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9154.435
-7.547240820D+05 1.251545253D+03 4.442424910D+00-9.786116430D-04 6.347511330D-07
-1.158320344D-10 6.870022460D-15                 9.318332700D+04 4.047521108D+00
ALCL2              Gurvich,1996a pt1 p171 pt2 p132.
 2 tpis96 AL  1.00CL  2.00    0.00    0.00    0.00 0   97.8875380    -240874.252
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12846.859
 5.340545950D+04-9.678057980D+02 1.006252671D+01-5.539528450D-03 5.823420560D-06
-3.306542450D-09 7.831562100D-13                -2.607627110D+04-2.393364216D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12846.859
 4.303453060D+05-1.552370585D+03 8.760657420D+00-9.467450060D-04 2.401844880D-07
-2.427836709D-11 8.390123470D-16                -2.145884709D+04-1.803641668D+01
ALCL3              Gurvich,1996a pt1 p173 pt2 p134.
 2 tpis96 AL  1.00CL  3.00    0.00    0.00    0.00 0  133.3405380    -584678.863
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16400.803
 7.750600970D+04-1.440779717D+03 1.401744141D+01-6.381631240D-03 5.871674720D-06
-2.908872278D-09 5.994050890D-13                -6.579343180D+04-4.494017799D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16400.803
-1.378630916D+05-5.579207290D+01 1.004190387D+01-1.682165339D-05 3.724664660D-09
-4.275526780D-13 1.982341329D-17                -7.343407470D+04-2.045130429D+01
ALF                Gurvich,1996a pt1 p151 pt2 p116.
 2 tpis96 AL  1.00F   1.00    0.00    0.00    0.00 0   45.9799412    -264060.446
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8892.107
 3.020771686D+04-3.080986949D+02 3.886413140D+00 3.564343690D-03-5.858471280D-06
 4.388109920D-09-1.256906273D-12                -3.117572862D+04 2.032567172D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8892.107
-7.111229050D+05 1.903013316D+03 2.191607179D+00 1.421471467D-03-4.179634770D-07
 6.153804400D-11-2.945403999D-15                -4.540728960D+04 1.613163743D+01
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Appendix D (*continued*)

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ALF+              Chase,1998 p92.
 2 j 6/76 AL  1.00F   1.00E  -1.00    0.00    0.00 0   45.9793926     692233.561
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8812.687
 3.643038120D+04-2.524634478D+02 3.105310486D+00 5.733270430D-03-8.839786990D-06
 6.343579590D-09-1.645011685D-12                 8.370237450D+04 6.764015580D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8812.687
 1.505101126D+06-2.236668821D+03 3.098216724D+00 3.115413930D-03-1.168427068D-06
 1.773587168D-10-9.665841380D-15                 9.885083850D+04 5.991894590D+00
ALFCL             Gurvich,1996a pt1 p182 pt2 p144.
 2 tpis96 AL  1.00F   1.00CL  1.00    0.00    0.00 0   81.4329412    -436409.913
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12133.195
 4.104779480D+04-5.769646420D+02 6.562642700D+00 4.106285840D-03-7.213921120D-06
 5.486401450D-09-1.580656193D-12                -5.114828700D+04-6.041227053D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12133.195
 6.970636350D+04-6.224485910D+02 7.573475410D+00-2.236155999D-04 2.382317949D-08
 4.443785760D-12-5.486977850D-16                -5.100943200D+04-1.091164505D+01
ALFCL2            Gurvich,1996a pt1 p183 pt2 p146.
 2 tpis96 AL  1.00F   1.00CL  2.00    0.00    0.00 0  116.8859412    -791395.404
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15738.260
 6.955607340D+04-1.188857902D+03 1.156672590D+01 4.574959490D-04-3.407372830D-06
 3.356822540D-09-1.085329228D-12                -9.162049260D+04-3.206065081D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15738.260
-1.720360526D+05-1.193340759D+02 1.008894431D+01-3.550993810D-05 7.830952610D-09
-8.961734230D-13 4.145330260D-17                -9.804185470D+04-2.127046859D+01
ALF2              Gurvich,1996a pt1 p153 pt2 p117.
 2 tpis96 AL  1.00F   2.00    0.00    0.00    0.00 0   64.9783444    -631764.175
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11600.932
 2.994951991D+04-2.194199915D+02 3.416748760D+00 1.272953936D-02-1.883312206D-05
 1.330702256D-08-3.680118630D-12                -7.607537650D+04 8.759626916D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11600.932
-2.146896245D+05 3.096840150D+01 6.816399620D+00 1.820129379D-04-7.793677440D-08
 1.472534201D-11-8.803695300D-16                -7.884002680D+04-7.915370474D+00
ALF2-             Gurvich,1996a pt1 p154 pt2 p118.
 2 tpis96 AL  1.00F   2.00E   1.00    0.00    0.00 0   64.9788930    -853230.685
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11331.815
 1.233369037D+05-1.348195504D+03 8.611178050D+00 2.245141297D-04-2.424673201D-06
 2.214132430D-09-6.602713960D-13                -9.708437460D+04-2.192617549D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11331.815
-1.590076965D+05-2.060486516D+02 7.155289380D+00-6.260167690D-05 1.391935746D-08
-1.603901265D-12 7.461508520D-17                -1.040479429D+05-1.122696648D+01
ALF2CL            Gurvich,1996a pt1 p182 pt2 p145.
 2 tpis96 AL  1.00F   2.00CL  1.00    0.00    0.00 0  100.4313444    -999128.145
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14827.517
 5.677412090D+04-8.869829470D+02 8.752746550D+00 8.195791200D-03-1.380480934D-05
 1.032703706D-08-2.948968416D-12                -1.177936778D+05-1.858347360D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14827.517
-2.115422988D+05-1.959188681D+02 1.014576850D+01-5.813219350D-05 1.281071982D-08
-1.465366277D-12 6.776002450D-17                -1.227153110D+05-2.359853398D+01
ALF3              Gurvich,1996a pt1 p157 pt2 p120.
 2 tpis96 AL  1.00F   3.00    0.00    0.00    0.00 0   83.9767476   -1209276.938
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14043.722
 4.410263520D+04-5.667495740D+02 5.833072850D+00 1.603535069D-02-2.413263602D-05
 1.714106160D-08-4.747543200D-12                -1.443349991D+05-5.461613658D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14043.722
-2.493972160D+05-2.911202519D+02 1.021662932D+01-8.642985970D-05 1.905713108D-08
-2.181058411D-12 1.009055287D-16                -1.475694276D+05-2.703983244D+01
ALF4-             Gurvich,1996a pt1 p159 pt2 p121.
 2 tpis96 AL  1.00F   4.00E   1.00    0.00    0.00 0  102.9756994   -1951600.806
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16786.835
 2.312010037D+05-3.235376780D+03 2.017865547D+01-9.108193500D-03 6.679552630D-06
-2.606075106D-09 4.110060510D-13                -2.211784563D+05-8.677268282D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16786.835
-3.217411610D+05-2.612097043D+02 1.319792654D+01-8.010135410D-05 1.786204421D-08
-2.062751964D-12 9.612581770D-17                -2.381577915D+05-4.231634322D+01
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ALH             Gurvich,1996a pt1 p139 pt2 p106.
 2 tpis96 AL  1.00H   1.00    0.00    0.00    0.00 0   27.9894780     249250.804
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8668.104
-3.759114030D+04 5.089002230D+02 1.128086896D+00 3.988660910D-03-2.150790303D-07
-2.176790819D-09 1.020805902D-12                 2.644431827D+04 1.650021856D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8668.104
 6.802018430D+06-2.178416933D+04 3.032713047D+01-1.503343597D-02 4.492142360D-06
-6.178450370D-10 3.115205260D-14                 1.658301221D+05-1.876766425D+02
ALHCL           Gurvich,1996a pt1 p178 pt2 p138.
 2 tpis96 AL  1.00H   1.00CL  1.00    0.00    0.00 0   63.4424780      10521.966
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10886.572
 3.587169760D+04-5.916249990D+02 6.944542380D+00-2.511543148D-03 6.471332550D-06
-5.642277140D-09 1.715950436D-12                 2.750930479D+03-9.903745880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10886.572
-1.683915330D+05-8.862301790D+02 8.062379400D+00-9.200551470D-04 3.949817220D-07
-6.401086760D-11 3.578354100D-15                 3.641504850D+03-1.800686894D+01
ALHCL2          Gurvich,1996a pt1 p179 pt2 p140.
 2 tpis96 AL  1.00H   1.00CL  2.00    0.00    0.00 0   98.8954780    -351278.965
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13676.196
 1.184828615D+05-2.054157118D+03 1.574696513D+01-1.476257296D-02 2.065336978D-05
-1.420198850D-08 3.826279860D-12                -3.434277460D+04-5.761184061D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13676.196
 9.608063940D+04-1.485540161D+03 1.103592709D+01-3.956955200D-04 8.465843730D-08
-9.483336520D-12 4.319033530D-16                 -3.669216390D+04-3.236862171D+01
ALHF            Gurvich,1996a pt1 p164 pt2 p125.
 2 tpis96 AL  1.00H   1.00F   1.00    0.00    0.00 0   46.9878812    -182614.484
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10572.121
-9.289545100D+03 1.335515868D+02 2.772448680D+00 6.751415030D-03-4.133846140D-06
 5.865704070D-10 2.276158011D-13                -2.384685845D+04 1.228752581D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10572.121
 7.342169250D+05-3.462164130D+03 1.039714588D+01-1.750737965D-03 4.615687860D-07
-5.390414740D-11 2.340478515D-15                -2.965279722D+03-3.713172313D+01
ALHFCL          Gurvich,1996a pt1 p184 pt2 p147.
 2 tpis96 AL  1.00H   1.00F   1.00CL  1.00    0.00 0   82.4408812    -555244.524
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12532.636
 1.290373237D+05-2.142099873D+03 1.485434420D+01-1.140326930D-02 1.564521768D-05
-1.067574855D-08 2.857255247D-12                -5.818303070D+04-5.483424986D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12532.636
 4.068987130D+04-1.502129854D+03 1.105214126D+01-4.031587730D-04 8.645252220D-08
-9.700659520D-12 4.423629510D-16                -6.129888110D+04-3.403564016D+01
ALHF2           Gurvich,1996a pt1 p166 pt2 p127.
 2 tpis96 AL  1.00H   1.00F   2.00    0.00    0.00 0   65.9862844    -765299.182
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12299.975
 1.050181431D+05-1.398654202D+03 9.166334840D+00 3.867286870D-03-4.830841090D-06
 3.099287181D-09-8.440702990D-13                -8.659048800D+04-2.557299683D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12299.975
-4.419947300D+03-1.612826324D+03 1.113336052D+01-4.351812660D-04 9.344396160D-08
-1.049431425D-11 4.788333980D-16                -8.606916190D+04-3.676383785D+01
ALH2            Gurvich,1996a pt1 p142 pt2 p107.
 2 tpis96 AL  1.00H   2.00    0.00    0.00    0.00 0   28.9974180     276774.934
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10090.834
 1.455182996D+04-2.153768996D+02 5.144370230D+00-3.965222030D-03 1.340900203D-05
-1.216744854D-08 3.743107130D-12                 3.311037940D+04-3.608799711D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10090.834
 1.432910601D+05-2.365907684D+03 9.085667190D+00-1.308536612D-03 4.777191360D-07
-7.324721890D-11 3.997900940D-15                 4.485951850D+04-3.220814285D+01
ALH2CL          Gurvich,1996a pt1 p179 pt2 p139.
 2 tpis96 AL  1.00H   2.00CL  1.00    0.00    0.00 0   64.4504180    -106345.406
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11253.251
 9.303828980D+04-1.328188016D+03 9.424763590D+00-3.277660590D-03 1.004231609D-05
-8.948123090D-09 2.708031665D-12                -7.647437930D+03-2.682512215D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11253.251
 3.166929930D+05-3.094037914D+03 1.215872020D+01-8.248269590D-04 1.765027123D-07
-1.977372723D-11 9.006176280D-16                 2.411845642D+03-4.718390855D+01
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Appendix D (*continued*)

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ALH2F              Gurvich,1996a pt1 p165 pt2 p126.
 2 tpis96 AL  1.00H   2.00F   1.00     0.00     0.00 0   47.9958212     -316655.854
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10764.801
 8.906039290D+04-9.750803930D+02 5.870772320D+00 6.896663690D-03-4.045817280D-06
 7.219318660D-10 7.329846740D-14                -3.425302600D+04-9.387539141D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10764.801
 2.711514962D+05-3.169623480D+03 1.221401118D+01-8.465600260D-04 1.812341995D-07
-2.030947985D-11 9.251825820D-16                -2.259217746D+04-4.941337333D+01
ALH3               Gurvich,1996a pt1 p145 pt2 p109.
 2 tpis96 AL  1.00H   3.00     0.00     0.00     0.00 0   30.0053580      128896.080
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10410.580
 1.481207909D+04-2.836495340D+01 2.507597126D+00 7.315920510D-03 2.331766687D-06
-6.389209890D-09 2.456885069D-12                1.463189428D+04 8.313187700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10410.580
 5.885458550D+05-4.595785660D+03 1.320893344D+01-1.226849004D-03 2.626580824D-07
-2.943725869D-11 1.341177648D-15                3.991716950D+04-6.181829295D+01
ALI                Gurvich,1996a pt1 p191 pt2 p153.
 2 tpis96 AL  1.00I   1.00     0.00     0.00     0.00 0  153.8860080      67395.017
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9751.117
 1.870854131D+03-1.543184003D+02 5.074391880D+00-1.120584830D-03 1.386302156D-06
-8.540782280D-10 2.180358492D-13                7.517443690D+03 6.688267622D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9751.117
 4.752817920D+05-1.198028588D+03 5.433685360D+00-1.004479306D-04-1.005928846D-07
 4.568173190D-11-3.960201360D-15                1.464627816D+04-3.141199746D+00
ALI2               Gurvich,1996a pt1 p193 pt2 p154.
 2 tpis96 AL  1.00I   2.00     0.00     0.00     0.00 0  280.7904780     -33812.954
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13923.046
 1.423413595D+04-4.646575690D+02 8.722674910D+00-3.560519290D-03 4.188682290D-06
-2.616026962D-09 6.720195510D-13               -3.846133330D+03-1.073076578D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13923.046
-3.355999020D+05 4.743347940D+02 7.106501390D+00-5.529965340D-04 3.161480314D-07
-5.515489160D-11 3.174155820D-15               -9.785488850D+03-5.602275944D-01
ALI3               Gurvich,1996a pt1 p195 pt2 p156.
 2 tpis96 AL  1.00I   3.00     0.00     0.00     0.00 0  407.6949480     -191330.433
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19003.567
 2.706032439D+04-7.559936810D+02 1.271396349D+01-5.466884090D-03 6.297618920D-06
-3.864209610D-09 9.774132440D-13               -2.220966921D+04-2.847883861D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19003.567
-6.357427470D+04-1.578772280D+01 1.001249733D+01-5.228673120D-06 1.196173520D-09
-1.409194490D-13 6.671276390D-18               -2.611455525D+04-1.247999813D+01
ALN                Gurvich,1996a pt1 p204 pt2 p164.
 2 tpis96 AL  1.00N   1.00     0.00     0.00     0.00 0   40.9882380      438829.011
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9265.111
 2.716645079D+04-2.543491110D+02 3.538987720D+00 5.296256160D-03-9.845700610D-06
 8.452209040D-09-2.592304568D-12                5.309994910D+04 5.399435220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9265.111
 3.821214220D+06-1.067776595D+04 1.449174222D+01-3.727227130D-03 7.922770960D-07
-8.086892210D-11 2.893539736D-15                1.205236340D+05-7.288585119D+01
ALO                Gurvich,1996a pt1 p122 pt2 p96.
 3 tpis96 AL  1.00O   1.00     0.00     0.00     0.00 0   42.9809380      67319.006
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8788.106
-7.683391100D+03 2.957969549D+02 4.808108440D-01 1.169224855D-02-1.595428871D-05
 1.060766814D-08-2.647888708D-12                5.843672170D+03 2.160997839D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8788.106
 1.565721161D+04 3.855741010D+03-5.926079780D+00 9.050960420D-03-2.930661549D-06
 4.238529070D-10-2.280655341D-14               -1.331694655D+04 6.830663436D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8788.106
 4.165661210D+07-3.768608760D+04 1.547867956D+01-9.568730340D-04 2.493109541D-08
 6.688940290D-14-8.998673700D-18                2.957786517D+05-9.427715804D+01
ALO+               Chase,1998 p133.
 2 j12/79 AL  1.00O   1.00E  -1.00     0.00     0.00 0   42.9803894      992993.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9089.716
 2.829178513D+04-4.179087100D+02 5.313299870D+00-1.410883046D-03 2.526524021D-06
-2.005474816D-09 5.762553550D-13                1.203648109D+05-3.410565930D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9089.716
 2.710846446D+04-6.998653420D+02 5.787815840D+00-6.871895460D-04 2.075047303D-07
-2.655281004D-11 1.283129660D-15                1.218682226D+05-7.051035880D+00
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ALO-              Gurvich,1996a pt1 p125 pt2 p98.
 2 g11/97 AL  1.00O   1.00E   1.00    0.00    0.00 0   42.9814866    -272921.782
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8744.718
 2.078075267D+04 2.859351226D+00 1.901912370D+00 7.301045660D-03-9.139769870D-06
 5.652983190D-09-1.396787103D-12                -3.359267730D+04 1.296339858D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8744.718
-6.971948290D+04-2.320553036D+02 4.672784330D+00-4.266447040D-05 1.632506336D-08
-1.727134051D-12 8.136840640D-17                -3.307718930D+04-2.155922595D+00
ALOCL             Gurvich,1996a pt1 p176 pt2 p136.
 2 tpis96 AL  1.00O   1.00CL  1.00    0.00    0.00 0   78.4339380    -301564.570
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11906.037
-5.144627790D+03-5.886297070D+01 4.452316930D+00 9.288235090D-03-1.246894823D-05
 8.178073540D-09-2.130739934D-12                -3.759683650D+04 2.476862818D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11906.037
-1.258027706D+05-2.420565961D+02 7.681130020D+00-7.268741700D-05 1.611337534D-08
 1.852889749D-12 8.607278220D-17                -3.754326050D+04-1.475818320D+01
ALOCL2            Gurvich,1996a pt1 p178 pt2 p137.
 2 tpis96 AL  1.00O   1.00CL  2.00    0.00    0.00 0  113.8869380    -402308.669
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15752.494
 6.902637130D+04-1.189297500D+03 1.161842739D+01 2.818279805D-04-3.145010615D-06
 3.168380650D-09-1.032375462D-12                -4.483323070D+04-3.165475132D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15752.494
-1.707713922D+05-1.180013804D+02 1.008798517D+01-3.513858040D-05 7.751187030D-09
-8.872470600D-13 4.104815440D-17                -5.124944140D+04-2.059252960D+01
ALOF              Gurvich,1996a pt1 p163 pt2 p123.
 2 tpis96 AL  1.00O   1.00F   1.00    0.00    0.00 0   61.9793412    -572289.603
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11003.003
 7.030578360D+03-1.154575430D+02 3.378823590D+00 1.283929158D-02-1.749748388D-05
 1.162605473D-08-3.064218613D-12                -6.959381700D+04 5.994804586D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11003.003
-1.641020297D+05-3.277770290D+02 7.744519740D+00-9.788649440D-05 2.165743208D-08
-2.486541919D-12 1.153633944D-16                -6.974085090D+04-1.717253748D+01
ALOF2             Gurvich,1996a pt1 p164 pt2 p124.
 2 tpis96 AL  1.00O   1.00F   2.00    0.00    0.00 0   80.9777444    -773649.771
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14055.387
 4.756085290D+04-6.124318360D+02 6.050223660D+00 1.559291479D-02-2.366136797D-05
 1.688366194D-08-4.690583100D-12                -9.171827490D+04-4.956258224D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14055.387
-2.496681413D+05-2.837821503D+02 1.021108125D+01-8.418303430D-05 1.855520828D-08
-2.122974022D-12 9.819319100D-17                -9.521804190D+04-2.522534812D+01
ALOF2-            Chase,1998 p98 6/76.
 2 g 2/01 AL  1.00O   1.00F   2.00E   1.00    0.00 0   80.9782930    -972289.619
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14076.981
 1.540605112D+05-1.928054597D+03 1.255806423D+01-4.904035370D-04-2.341783347D-06
 2.415138600D-09-7.471809250D-13                -1.091430174D+05-4.265821750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14076.981
-2.389881459D+05-2.880143725D+02 1.021700240D+01-8.747062000D-05 1.944846334D-08
-2.241045051D-12 1.042591053D-16                -1.190576566D+05-2.600779629D+01
ALOH              Gurvich,1996a pt1 p145 pt2 p110.
 2 tpis96 AL  1.00O   1.00H   1.00    0.00    0.00 0   43.9888780    -192762.171
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10351.931
 5.876493180D+04-9.449422690D+02 7.820599180D+00 5.858888470D-04-4.083666810D-06
 4.587229340D-09-1.563936726D-12                -1.993283011D+04-2.065043885D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10351.931
 7.882068110D+05-2.263671626D+03 7.823954880D+00 1.821171456D-04-8.263729320D-08
 1.265414876D-11-6.875972530D-16                -1.039808093D+04-2.209032458D+01
ALOHCL            Gurvich,1996a pt1 p180 pt2 p141.
 2 tpis96 AL  1.00O   1.00H   1.00CL  1.00    0.00    0.00 0   79.4418780    -373785.740
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13918.918
 1.636360341D+04-1.915959416D+02 4.711170470D+00 1.388068475D-02-1.999018454D-05
 1.439647350D-08-4.033330450D-12                -4.568083720D+04 4.644207506D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13918.918
 7.967115510D+05-2.843470502D+03 1.095559970D+01-1.099328162D-04-1.344506283D-08
 4.415893770D-12-2.973546112D-16                -2.969861461D+04-3.296113996D+01
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ALOHCL2           Gurvich,1996a pt1 p181 pt2 p143.
 2 tpis96 AL  1.00O   1.00H   1.00CL  2.00    0.00 0  114.8948780    -725145.408
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17149.806
 3.971929860D+04-7.751554960D+02 9.494051530D+00 1.074401359D-02-1.676464791D-05
 1.259706368D-08-3.613177980D-12                -8.584796930D+04-1.993481642D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17149.806
 7.385929760D+05-2.863204228D+03 1.397062327D+01-1.160311527D-04-1.208248796D-08
 4.258327630D-12-2.900049181D-16                -7.293048000D+04-4.681834857D+01
ALOHF             Gurvich,1996a pt1 p166 pt2 p128.
 2 tpis96 AL  1.00O   1.00H   1.00F   1.00    0.00 0   62.9872812    -574211.575
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13315.081
-1.556003336D+03 2.886581999D+02 7.703793290D-01 2.450406329D-02-3.417811010D-05
 2.388932902D-08-6.570480510D-12                -7.177222560D+04 2.453071801D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13315.081
 7.557113130D+05-2.936702803D+03 1.102455104D+01-1.373078030D-04-7.432816160D-09
 3.729981220D-12-2.657027781D-16                -5.340130900D+04-3.527397302D+01
ALOHF2            Gurvich,1996a pt1 p168 pt2 p130.
 2 tpis96 AL  1.00O   1.00H   1.00F   2.00    0.00 0   81.9856844   -1141510.711
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15428.498
 1.738263538D+04-1.307687299D+02 3.312381920D+00 2.784734099D-02-3.982363210D-05
 2.809344456D-08-7.764574200D-12                -1.384133568D+05 1.004739945D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15428.498
 6.530119920D+05-3.034017232D+03 1.409719788D+01-1.663681799D-04-1.011564183D-09
 2.993805003D-12-2.315956955D-16                -1.223052213D+05-5.151210690D+01
ALO2              Gurvich,1996a pt1 p126 pt2 p99.
 2 tpis96 AL  1.00O   2.00    0.00    0.00    0.00 0   58.9803380     -38657.871
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13361.629
 4.338480450D+04-4.735292260D+02 6.001717670D+00 7.094420880D-03-1.129107996D-05
 8.252691680D-09-2.327652976D-12                -3.826145800D+03-4.830022480D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13361.629
 1.187216642D+05-8.335625400D+02 8.309301190D+00-3.538667220D-04 5.967069460D-08
 4.014897700D-14-3.515702520D-16                -2.033107586D+03-1.715063884D+01
ALO2-             Gurvich,1996a pt1 p128 pt2 p100.
 2 tpis96 AL  1.00O   2.00E   1.00    0.00    0.00 0   58.9808866     -452572.223
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10644.677
 1.178678641D+05-1.507186304D+03 9.524749750D+00-5.207989020D-04-1.586902345D-06
 1.700455028D-09-5.301419770D-13                -4.825469270D+04-3.081215859D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10644.677
-1.872410758D+05-2.338853263D+02 7.676070020D+00-7.093570300D-05 1.576717569D-08
-1.816494162D-12 8.449707960D-17                -5.594640560D+04-1.773751567D+01
AL(OH)2           Gurvich,1996a pt1 p149 pt2 p113.
 2 tpis96 AL  1.00O   2.00H   2.00    0.00    0.00 0   60.9962180     -507660.670
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14027.535
 4.397316910D+03 1.327680339D+02 1.093947024D+00 3.054059173D-02-4.375943350D-05
 3.174617430D-08-9.004259400D-12                -6.315437390D+04 2.101977655D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14027.535
 1.669643735D+06-5.924738280D+03 1.549480264D+01-5.383488080D-04 5.413044530D-08
-1.196022328D-12-1.082001733D-16                -2.697525061D+04-6.617911543D+01
AL(OH)2CL         Gurvich,1996a pt1 p181 pt2 p142.
 2 tpis96 AL  1.00O   2.00H   2.00CL  1.00    0.00 0   96.4492180     -859056.724
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17222.037
 2.477879709D+04-4.454577210D+02 5.928470200D+00 2.730162734D-02-4.041405370D-05
 2.974210410D-08-8.477150600D-12                -1.033778030D+05-3.679940779D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17222.037
 1.603911487D+06-5.767232240D+03 1.817772266D+01-3.691816150D-04 1.137918702D-08
 4.083079400D-12-3.641323430D-16                -7.118699850D+04-7.757541774D+01
AL(OH)2F          Gurvich,1996a pt1 p167 pt2 p129.
 2 tpis96 AL  1.00O   2.00H   2.00F   1.00    0.00 0   79.9946212    -1069628.708
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16472.051
 2.132812662D+04-1.932900224D+02 3.069174664D+00 3.555017330D-02-5.181158330D-05
 3.753520280D-08-1.059220701D-11                -1.295797992D+05 1.001897011D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16472.051
 1.559238236D+06-5.841273030D+03 1.823229919D+01-3.907805420D-04 1.610928938D-08
 3.544784060D-12-3.393453880D-16                -9.623100890D+04-7.971351802D+01
```

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AL(OH)3             Gurvich,1996a pt1 p150 pt2 p115.
 2 tpis96 AL  1.00O   3.00H   3.00    0.00    0.00 0   78.0035580   -1012667.542
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17594.767
-1.402475452D+04 3.696073460D+02-2.979600650D-01 4.929859350D-02-6.981572280D-05
 5.014801700D-08-1.412480165D-11                -1.255260760D+05 2.711490074D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17594.767
 2.477063616D+06-8.968617250D+03 2.280320998D+01-8.320292250D-04 8.663494430D-08
-2.420287082D-12-1.331746442D-16                -7.015278640D+04-1.121899198D+02
ALS                 Gurvich,1996a pt1 p197 pt2 p158.
 2 tpis96 AL  1.00S   1.00    0.00    0.00    0.00 0   59.0465380     232682.009
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9088.109
 2.611742801D+04-3.470673890D+02 4.436204590D+00 3.340168210D-03-8.410199670D-06
 8.508185110D-09-2.780868507D-12                 2.863779062D+04 7.522705491D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9088.109
 8.909844290D+06-2.507677454D+04 2.893456134D+01-9.839766820D-03 2.045319809D-06
-2.087970890D-10 8.152792520D-15                 1.885761615D+05-1.786036457D+02
ALS2                Gurvich,1996a pt1 p198 pt2 p159.
 2 tpis96 AL  1.00S   2.00    0.00    0.00    0.00 0   91.1115380     248535.279
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14428.779
 4.252335410D+04-7.764603300D+02 9.801068960D+00-3.910680090D-03 3.875695970D-06
-2.082025593D-09 4.682935890D-13                 3.167961540D+04-2.178097896D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14428.779
-6.852563540D+04-2.671667739D+01 7.520193860D+00-8.148565100D-06 1.811865152D-09
-2.086958125D-13 9.703246380D-18                 2.758362737D+04-7.873490263D+00
AL2                 Gurvich,1996a pt1 p118 pt2 p95.
 2 tpis96 AL  2.00    0.00    0.00    0.00    0.00 0   53.9630760     501301.722
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10139.122
-5.281509650D+03-1.727374523D+01 4.604077010D+00-2.616467770D-04 6.302319970D-07
-3.290938590D-10 8.888365140D-14                 5.900706390D+04 3.060188921D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10139.122
-2.320724102D+06 9.218707890D+03-9.446951870D+00 9.999920010D-03-3.154798085D-06
 4.361544810D-10-2.241157240D-14                 2.904589544D+03 9.960320745D+01
AL2Br6              Gurvich,1996a pt1 p190 pt2 p152.
 2 tpis96 AL  2.00BR  6.00    0.00    0.00    0.00 0  533.3870760    -942422.811
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        38217.189
 6.483319700D+04-1.947687811D+03 2.886989822D+01-1.365825785D-02 1.557883731D-05
-9.486942000D-09 2.385519396D-12                -1.101526833D+05-1.025934782D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        38217.189
-1.731829490D+05-4.342299780D+01 2.203414210D+01-1.421187503D-05 3.238631340D-09
-3.803879760D-13 1.796525455D-17                -1.202338355D+05-6.201054950D+01
AL2C2               Gurvich,1996a pt1 p206 pt2 p167.
 2 tpis96 AL  2.00C   2.00    0.00    0.00    0.00 0   77.9844760     544978.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16165.001
 1.110987147D+04-3.502434230D+02 8.598856000D+00 1.832528671D-03 1.035743392D-06
-2.091649890D-09 7.716068700D-13                 6.492764190D+04-1.645080239D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16165.001
 1.597651967D+05-1.644007203D+03 1.164643675D+01-4.379215430D-04 9.369640110D-08
-1.049615854D-11 4.780468930D-16                 7.204889810D+04-3.648164252D+01
AL2CL6              Gurvich,1996a pt1 p175 pt2 p135.
 2 tpis96 AL  2.00CL  6.00    0.00    0.00    0.00 0  266.6810760   -1296876.242
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        34147.090
 1.340935279D+05-3.001037953D+03 3.143000879D+01-1.700408496D-02 1.786540089D-05
-1.015419943D-08 2.409630451D-12                -1.471830046D+05-1.274445324D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        34147.090
-2.752975554D+05-9.248235970D+01 2.207058224D+01-2.870537915D-05 6.423325690D-09
-7.436585200D-13 3.472064670D-17                -1.629157014D+05-7.091602129D+01
AL2F6               Gurvich,1996a pt1 p160 pt2 p122.
 2 tpis96 AL  2.00F   6.00    0.00    0.00    0.00 0  167.9534952   -2632491.231
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26064.089
 1.915061289D+05-3.168240250D+03 2.245374802D+01 1.271532036D-02-2.488697302D-05
 1.955252096D-08-5.712084890D-12                -3.049962550D+05-9.396473101D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26064.089
-5.852982610D+05-5.450571990D+02 2.240686320D+01-1.627323704D-04 3.595225040D-08
-4.121201440D-12 1.909095384D-16                -3.219683910D+05-8.589867941D+01
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Appendix D (*continued*)

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AL2I6             Gurvich,1996a pt1 p196 pt2 p157.
 2 tpis96 AL  2.00I   6.00    0.00    0.00    0.00 0  815.3898960    -487747.035
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        40920.966
 2.587571514D+04-1.280719742D+03 2.677715820D+01-9.913018470D-03 1.168760413D-05
-7.303918530D-09 1.874532749D-12                -5.891105550D+04-8.330209321D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        40920.966
-1.210112399D+05-2.467542774D+01 2.201992650D+01-8.462022590D-06 1.957831901D-09
-2.326573151D-13 1.108910373D-17                -6.548523750D+04-5.528536481D+01
AL2O              Gurvich,1996a pt1 p129 pt2 p101.
 2 tpis96 AL  2.00O   1.00    0.00    0.00    0.00 0   69.9624760    -148611.286
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12776.514
 7.776530700D+03-1.294235361D+02 4.912509520D+00 8.604223450D-03-1.217703648D-05
 8.314634870D-09-2.237722201D-12                -1.886512879D+04-2.806368311D-02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12776.514
-1.171074351D+05-1.783009166D+02 7.633215360D+00-5.335931770D-05 1.180702791D-08
-1.355444579D-12 6.287323890D-17                -1.947580149D+04-1.415764167D+01
AL2O+             Chase,1998 p151 12/79.
 2 g 1/01 AL  2.00O   1.00E  -1.00    0.00    0.00 0   69.9619274     648970.248
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12981.148
 6.828925720D+04-9.098504170D+02 8.896563010D+00-7.772554380D-04-4.034655620D-07
 6.977315050D-10-2.417262484D-13                 8.085007550D+04-2.176216731D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12981.148
-1.102225105D+05-1.214571732D+02 7.591595950D+00-3.694539160D-05 8.218520320D-09
-9.473649720D-13 4.408621350D-17                 7.614943580D+04-1.282233856D+01
AL2O2             Gurvich,1996a pt1 p131 pt2 p102.
 2 tpis96 AL  2.00O   2.00    0.00    0.00    0.00 0   85.9618760    -403095.587
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15842.613
-1.940560042D+04 2.508489836D+02 3.621403790D+00 1.951385302D-02-2.560329071D-05
 1.662721576D-08-4.312396200D-12                -5.172697280D+04 9.923995945D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15842.613
-1.940611656D+05-4.609752430D+02 1.084375637D+01-1.376042893D-04 3.044733119D-08
-3.496193920D-12 1.622305079D-16                -4.963055780D+04-2.946538090D+01
AL2O2+            Chase,1998 p153 12/79.
 2 g 2/01 AL  2.00O   2.00E  -1.00    0.00    0.00 0   85.9613274     557438.835
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14975.135
 8.292034990D+04-1.757427015D+03 1.525328567D+01-8.983131330D-03 8.953954500D-06
-4.840586200D-09 1.096696856D-12                 7.311677140D+04-5.517092550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14975.135
-1.652005184D+05-6.021606970D+01 1.004626917D+01-1.892194088D-05 4.253301200D-09
-4.942390420D-13 2.314507373D-17                 6.386219000D+04-2.345753361D+01
AL2O3             Gurvich,1996a pt1 p137 pt2 p105.
 2 tpis96 AL  2.00O   3.00    0.00    0.00    0.00 0  101.9612760    -546890.530
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19598.070
-7.443374320D+03 8.829004210D+01 5.264662640D+00 2.507678848D-02-3.434541650D-05
 2.302516980D-08-6.122529280D-12                -6.872685950D+04 2.202324298D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19598.070
-2.777784969D+05-4.917465930D+02 1.386703888D+01-1.469381940D-04 3.250406490D-08
-3.730867350D-12 1.730444284D-16                -6.790757850D+04-4.375559873D+01
AL2S              Gurvich,1996a pt1 p199 pt2 p160.
 2 tpis96 AL  2.00S   1.00    0.00    0.00    0.00 0   86.0280760     220679.131
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14003.931
 4.094624370D+04-7.797172470D+02 9.814423100D+00-3.940339820D-03 3.912465430D-06
-2.105891677D-09 4.746001080D-13                 2.833963305D+04-2.465067552D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14003.931
-7.043437370D+04-2.676376869D+01 7.520233820D+00-8.166123060D-06 1.816026040D-09
-2.091989298D-13 9.727537700D-18                 2.422718377D+04-1.066580982D+01
AL2S2             Gurvich,1996a pt1 p200 pt2 p161.
 2 tpis96 AL  2.00S   2.00    0.00    0.00    0.00 0  118.0930760     135287.321
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18099.521
 6.614587320D+04-1.111319537D+03 1.257007304D+01-1.456053256D-03-5.851627110D-07
 1.390055053D-09-5.496468200D-13                 1.914456895D+04-3.600277092D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18099.521
-1.377806456D+05-7.705032500D+01 1.055723566D+01-2.277554487D-05 5.007682850D-09
-5.715862120D-13 2.637999240D-17                 1.313336091D+04-2.256851594D+01
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Ar                Ref-Elm. Moore,1971. Gordon,1999.
 3 g 3/98 AR  1.00    0.00    0.00    0.00    0.00 0   39.9480000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 4.379674910D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.010538475D+01-5.992661070D-02 2.500069401D+00-3.992141160D-08 1.205272140D-11
-1.819015576D-15 1.078576636D-19                -7.449939610D+02 4.379180110D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-9.951265080D+08 6.458887260D+05-1.675894697D+02 2.319933363D-02-1.721080911D-06
 6.531938460D-11-9.740147729D-16                -5.078300340D+06 1.465298484D+03
Ar+               Moore,1971. IP:Moore,1970a. Gordon,1999.
 3 g 1/99 AR  1.00E  -1.00    0.00    0.00    0.00 0   39.9474514    1526778.407
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6205.988
-5.731209170D+04 7.930791470D+02-1.717121217D+00 1.044184018D-02-1.180207501D-05
 6.528134780D-09-1.447558130D-12                 1.790572230D+05 2.949150950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6205.988
-3.835965400D+05 8.162019700D+02 2.301342628D+00-4.952983770D-06 1.205108477D-08
-2.185050286D-12 1.265493898D-16                 1.771811455D+05 7.947507480D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6205.988
 1.006884827D+07-6.624361280D+03 4.446908200D+00-3.017567664D-04 2.612882069D-08
-1.201637769D-12 2.299206903D-17                 2.349504137D+05-1.032262257D+01
B                 Martin,1998. Odintzova,1979. Gordon,1999.
 3 g 9/98 B   1.00    0.00    0.00    0.00    0.00 0   10.8110000     575598.760
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6316.060
 1.182394638D+02-7.009916910D-02 2.500236159D+00-4.584213700D-07 5.123185830D-10
-3.057217674D-13 7.533815325D-17                 6.848359080D+04 4.209501920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6316.060
-1.072659610D+05 3.225307160D+02 2.126407232D+00 2.106579339D-04-5.937129160D-08
 7.377427990D-12-2.282443381D-16                 6.643413100D+04 6.877069670D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6316.060
-4.150001310D+08 2.329576796D+05-4.720913710D+01 4.877655960D-03-2.069413791D-07
 3.233519090D-12-1.824076527D-18                -1.802904743D+06 4.439617640D+02
B+                Moore,1971. IP:Moore,1970a. Gordon,1999.
 3 g 9/98 B   1.00E  -1.00    0.00    0.00    0.00 0   10.8104514    1382315.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 7.849791190D-02-8.947480950D-04 2.500004085D+00-9.577271230D-09 1.218136411D-11
-7.986752520D-15 2.113769829D-18                 1.655080260D+05 2.419053631D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-8.911548030D+03 4.587790090D+00 2.531500086D+00-4.903949100D-05 2.853326582D-08
-7.382175910D-12 7.120721560D-16                 1.654526303D+05 2.238669780D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-7.977322890D+08 4.734044940D+05-1.055286044D+02 1.170310076D-02-6.075531110D-07
 1.484174716D-11-1.328323987D-16                -3.609116960D+06 9.497399750D+02
B-                Hotop,1985. Gordon,1999.
 3 g 9/98 B   1.00E   1.00    0.00    0.00    0.00 0   10.8115486     542631.498
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6272.598
 2.201568105D+01-4.740468880D-03 2.500014238D+00-2.497056599D-08 2.556360708D-11
-1.415274780D-14 3.271770710D-18                 6.451791880D+04 4.616367290D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6272.598
 2.118018248D+01 2.070697496D-04 2.499999729D+00 1.456693631D-10-3.888571760D-14
 5.090598630D-18-2.601566168D-22                 6.451789140D+04 4.616455830D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6272.598
-1.311386485D+02 9.028908800D-02 2.499978572D+00 2.606391052D-09-1.716068068D-13
 5.810865540D-18-7.925029090D-23                 6.451717400D+04 4.616640300D+00
BBr               Gurvich,1996a pt1 p91 pt2 p70.
 2 g 9/98 B   1.00BR  1.00    0.00    0.00    0.00 0   90.7150000     240952.358
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8997.058
 3.796093500D+04-4.976096020D+02 5.267008200D+00-3.742840190D-05-1.131544370D-06
 1.261945702D-09-4.288811880D-13                 3.038125367D+04-4.353407330D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8997.058
 2.536858027D+05-6.405909500D+02 4.666823470D+00 4.175486390D-04-2.963714868D-07
 7.519119540D-11-4.835368320D-15                 3.189084340D+04-8.255870910D-01
BBr2              Gurvich,1996a pt1 p92 pt2 p71.
 2 g 9/98 B   1.00BR  2.00    0.00    0.00    0.00 0  170.6190000      97828.617
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12200.717
 6.516550710D+04-9.029590760D+02 8.063817800D+00 1.129849010D-03-4.195482390D-06
 3.965658770D-09-1.283029835D-12                 1.470466408D+04-1.336453164D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12200.717
-4.191633370D+05 4.157688470D+02 7.148169830D+00-5.689590750D-04 3.195441770D-07
-5.553176990D-11 3.191136760D-15                 6.118982050D+03-5.502759620D+00
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Appendix D (*continued*)

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BBr3                Gurvich,1996a pt1 p93 pt2 p72.
 2 tpis96 B   1.00BR  3.00    0.00    0.00    0.00 0  250.5230000    -205300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15702.797
 3.968073690D+04-6.331087160D+02 8.054551570D+00 9.777571300D-03-1.614866025D-05
 1.216119883D-08-3.516539610D-12                -2.366723308D+04-1.106099390D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15702.797
-1.901046795D+05-1.503627687D+02 1.010999896D+01-4.323095110D-05 9.409696190D-09
-1.065218470D-12 4.883048770D-17                -2.742553062D+04-1.997496003D+01
BC                  Gurvich,1996a pt1 p108 pt2 p86.
 2 g 9/98 B   1.00C   1.00    0.00    0.00    0.00 0   22.8217000     838161.905
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8735.105
-3.915758000D+04 7.284538060D+02-1.552743361D+00 1.552898673D-02-1.976857863D-05
 1.272066405D-08-3.229982780D-12                 9.644913680D+04 3.248204466D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8735.105
-2.346280674D+06 6.450751300D+03-2.619532384D+00 3.339160500D-03-4.508022140D-07
 1.351919576D-11 8.265104270D-16                 5.786685070D+04 5.037884876D+01
BC2                 Gurvich,1996a pt1 p109 pt2 p87.
 2 g 9/98 B   1.00C   2.00    0.00    0.00    0.00 0   34.8324000     801258.725
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11687.825
-2.987422175D+04 3.643126580D+02 2.963469415D+00 6.561750150D-03-3.539767240D-06
 1.927356029D-10 3.118724866D-13                 9.304835730D+04 1.083424193D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11687.825
 1.525485889D+06-5.987862380D+03 1.408384855D+01-3.747499800D-03 1.081927223D-06
-1.378744645D-10 6.473822000D-15                 1.311204013D+05-6.337215498D+01
BCL                 Gurvich,1996a pt1 p73 pt2 p51.
 2 g 9/98 B   1.00CL  1.00    0.00    0.00    0.00 0   46.2640000     183173.437
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8861.337
 2.202458989D+04-1.700511155D+02 3.066075869D+00 5.595070180D-03-8.460870410D-06
 6.084733410D-09-1.702889433D-12                 2.197402537D+04 6.388978917D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8861.337
-7.421262540D+04 2.638090127D+02 3.600227650D+00 1.018866266D-03-4.666184120D-07
 9.849002030D-11-6.468818170D-15                 1.912726480D+04 5.235317877D+00
BCL+                Chase,1998 p198.
 2 j 6/68 B   1.00CL  1.00E  -1.00    0.00    0.00 0   46.2634514    1234280.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8860.318
 6.514405420D+04-6.845541010D+02 5.527276820D+00-4.458357450D-04-4.557728840D-07
 6.370858160D-10-2.134366120D-13                 1.509424507D+05-6.918246393D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8860.318
-2.169423542D+05 3.589975160D+02 4.035208370D+00 3.274452430D-04-8.634578450D-08
 1.207061044D-11-5.262253270D-16                 1.445477224D+05 3.488222017D+00
BCLOH               Gurvich,1996a pt1 p83 pt2 p61.
 2 g 9/98 B   1.00CL  1.00O   1.00H   1.00    0.00 0   63.2713400    -234005.381
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12431.519
-2.898427288D+04 6.894046580D+02-2.288138069D+00 3.349428620D-02-4.725225980D-05
 3.326981310D-08-9.224238860D-12                -3.261981100D+04 3.976886651D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12431.519
 7.027738440D+05-2.857391274D+03 1.091175840D+01-8.107709340D-05-2.124440337D-08
 5.409912440D-12-3.464153840D-16                -1.307221888D+04-3.585168799D+01
BCL(OH)2            Gurvich,1996a pt1 p85 pt2 p62.
 2 tpis96 B   1.00CL  1.00O   2.00H   2.00    0.00 0   80.2786800    -805387.658
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13565.103
 8.072623010D+04-8.594619820D+02 2.705039614D+00 3.878799620D-02-5.721734350D-05
 4.145850330D-08-1.168536754D-11                -9.379910740D+04 7.134982695D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13565.103
 1.423878191D+06-5.849704070D+03 1.792165219D+01-2.009909087D-04-3.393435780D-08
 9.838560760D-12-6.472678820D-16                -6.474261760D+04-8.100399519D+01
BCL2                Gurvich,1996a pt1 p74 pt2 p52.
 2 tpis96 B   1.00CL  2.00    0.00    0.00    0.00 0   81.7170000     -60881.490
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11513.621
 3.598879420D+04-3.602826500D+02 4.157685450D+00 1.152877450D-02-1.816567395D-05
 1.341714418D-08-3.840822860D-12                -6.765107050D+03 5.182311874D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11513.621
 3.501403130D+05-1.662203590D+03 8.839534720D+00-9.772544110D-04 2.467356248D-07
-2.501151018D-11 8.722954560D-16                 5.682909440D+02-2.148348344D+01
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BCL2+              Chase,1998 p203 12/79.
 2 g 1/01 B   1.00CL  2.00E  -1.00    0.00    0.00 0   81.7164514     672315.402
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12848.802
 8.065956240D+04-1.149602601D+03 1.016765297D+01-3.586494910D-03 2.837145924D-06
-1.225075731D-09 2.224794198D-13                 8.478617410D+04-2.937256994D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12848.802
 3.029293331D+05-1.305533159D+03 8.920390060D+00-7.289919640D-04 1.727833266D-07
-1.523567337D-11 4.226911440D-16                 8.653415770D+04-2.267466616D+01
BCL2OH             Gurvich,1996a pt1 p86 pt2 p63.
 2 tpis96 B   1.00CL  2.00O   1.00H   1.00    0.00 0   98.7243400    -604917.444
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14051.769
 2.099755170D+04-2.470699169D+02 2.578761742D+00 3.120362393D-02-4.545314050D-05
 3.242011770D-08-9.039822660D-12                -7.309028620D+04 1.273658611D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14051.769
 5.878113790D+05-2.982969317D+03 1.400662004D+01-1.194189832D-04-1.269775742D-08
 4.422892190D-12-3.004089365D-16                -5.824168070D+04-5.150858228D+01
BCL3               Gurvich,1996a pt1 p76 pt2 p53.
 2 tpis96 B   1.00CL  3.00    0.00    0.00    0.00 0  117.1700000    -404500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13970.666
 2.392970339D+04-4.140378860D+02 5.488035260D+00 1.648395682D-02-2.456196216D-05
 1.743876340D-08-4.845222140D-12                -4.839469840D+04-1.675355198D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13970.666
-2.417408819D+05-2.921539509D+02 1.021668480D+01-8.623637100D-05 1.897792088D-08
-2.168726841D-12 1.002154013D-16                -5.074834440D+04-2.546862377D+01
BF                 Gurvich,1996a pt1 p56 pt2 p36.
 2 g10/97 B   1.00F   1.00    0.00    0.00    0.00 0   29.8094032    -106931.884
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8694.670
-5.238954730D+04 8.118476640D+02-1.141614903D+00 1.161249417D-02-1.175212617D-05
 6.019232780D-09-1.238293129D-12                -1.774541998D+04 3.005086287D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8694.670
-3.746389780D+05 5.604493910D+02 3.609186110D+00 6.187216930D-04-1.778938770D-07
 2.426601527D-11-9.394651580D-16                -1.819179292D+04 3.716609290D+00
BFCL               Gurvich,1996a pt1 p86 pt2 p64.
 2 tpis96 B   1.00F   1.00CL  1.00    0.00    0.00 0   65.2624032    -279184.068
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11033.040
-2.363512735D+04 4.383168980D+02 3.918095720D-01 1.719990692D-02-2.139592424D-05
 1.337389186D-08-3.371164690D-12                -3.687166590D+04 2.668102752D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11033.040
-1.086309561D+05-5.233438480D+02 7.297504740D+00-3.054410701D-05-3.154598306D-08
 1.052290533D-11-7.615432260D-16                -3.305891210D+04-1.186586595D+01
BFCL2              Gurvich,1996a pt1 p88 pt2 p66.
 2 tpis96 B   1.00F   1.00CL  2.00    0.00    0.00 0  100.7154032    -643000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.913
 4.402551240D+03-1.571398929D+02 4.016322310D+00 1.743396078D-02-2.252789060D-05
 1.433673443D-08-3.648755580D-12                -7.822452620D+04 6.886094746D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.913
-2.233613309D+05-6.440602960D+02 1.047861848D+01-1.911892367D-04 4.224887790D-08
-4.847266920D-12 2.247974725D-16                -7.740626480D+04-2.814630564D+01
BFOH               Gurvich,1996a pt1 p71 pt2 p48.
 2 g 9/98 B   1.00F   1.00O   1.00H   1.00    0.00 0   46.8167432    -451631.678
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11973.122
-7.563953670D+04 1.354838128D+03-5.648210110D+00 3.870274660D-02-5.037659180D-05
 3.339592640D-08-8.847822950D-12                -6.194446110D+04 5.800362820D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11973.122
 7.251318090D+05-3.215620850D+03 1.117909777D+01-1.883881929D-04 2.579708080D-09
 2.665158100D-12-2.186647438D-16                -3.716808080D+04-3.978463490D+01
BF(OH)2            Gurvich,1996a pt1 p71 pt2 p49.
 2 tpis96 B   1.00F   1.00O   2.00H   2.00    0.00 0   63.8240832   -1049889.539
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12885.220
 1.381800676D+04 2.529637004D+02-3.844552040D+00 5.255140850D-02-7.193117730D-05
 4.948309910D-08-1.345922496D-11                -1.283123258D+05 4.293659370D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12885.220
 1.422037640D+06-6.257297570D+03 1.822460686D+01-3.221396450D-04-7.126739900D-09
 6.758699770D-12-5.042554540D-16                -9.186254190D+04-8.527895050D+01
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Appendix D (*continued*)

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BF2                Gurvich,1996a pt1 p58 pt2 p37.
 2 tpis96 B   1.00F   2.00    0.00    0.00    0.00 0   48.8078064    -499426.904
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10612.202
-6.787651760D+04 1.085903536D+03-3.023320961D+00 2.326503687D-02-2.641444147D-05
 1.515620683D-08-3.518559180D-12                -6.640918250D+04 4.431968310D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10612.202
-1.153091296D+05-8.109800120D+02 7.602709230D+00-2.409209242D-04 5.328471860D-08
-6.118797940D-12 2.839984178D-16                -5.796222170D+04-1.655644047D+01
BF2+               Chase,1998 p211.
 2 j12/70 B   1.00F   2.00E  -1.00    0.00    0.00 0   48.8072578     322586.400
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10612.483
-2.938356477D+04 2.955698598D+02 1.894274526D+00 1.280508319D-02-1.388757254D-05
 7.624366750D-09-1.706339371D-12                 3.598992440D+04 1.384803311D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10612.483
-1.769409966D+05-5.343685180D+02 7.728052910D+00-1.958622052D-06-2.419680893D-08
 5.732533810D-12-3.216354230D-16                 3.908745050D+04-1.936560315D+01
BF2-               Gurvich,1996a pt1 p60 pt2 p38.
 2 tpis96 B   1.00F   2.00E   1.00    0.00    0.00 0   48.8083550    -733802.963
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10433.571
 2.109765318D+04 1.439564600D+02 2.604646296D-01 1.817373751D-02-2.241565287D-05
 1.369712886D-08-3.355952680D-12                -8.971801780D+04 2.351692604D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10433.571
-1.709920627D+05-6.156219790D+02 7.458871370D+00-1.836703248D-04 4.064363960D-08
-4.667700950D-12 2.166264840D-16                -8.741404530D+04-1.620604664D+01
BF2CL              Gurvich,1996a pt1 p87 pt2 p65.
 2 tpis96 B   1.00F   2.00CL  1.00    0.00    0.00 0   84.2608064    -888000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12323.693
 4.500101250D+03-1.196284966D+02 3.198635140D+00 1.743426933D-02-1.994070287D-05
 1.125136430D-08-2.544020371D-12                -1.076779851D+05 1.008195015D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12323.693
-2.066817398D+05-1.024447292D+03 1.075843981D+01-3.023235319D-04 6.672521470D-08
-7.649941900D-12 3.546224500D-16                -1.046936725D+05-3.229995036D+01
BF2OH              Gurvich,1996a pt1 p72 pt2 p50.
 2 tpis96 B   1.00F   2.00O   1.00H   1.00    0.00 0   65.8151464    -1092217.322
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12395.887
-7.522521650D+03 4.367121690D+02-3.128973474D+00 4.323957680D-02-5.785494040D-05
 3.885858130D-08-1.038574523D-11                -1.344259458D+05 4.139170550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12395.887
 5.760759250D+05-3.611900190D+03 1.446897640D+01-3.028293733D-04 2.764337508D-08
-1.905493170D-13-8.694971940D-17                -1.133589041D+05-5.896981510D+01
BF3                Gurvich,1996a pt1 p62 pt2 p39.
 2 tpis96 B   1.00F   3.00    0.00    0.00    0.00 0   67.8062096    -1136000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11651.226
 3.465584000D+03 2.133198651D+01 1.641245191D+00 1.993755064D-02-2.150119930D-05
 1.145669081D-08-2.442285789D-12                -1.379455591D+05 1.625533544D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11651.226
-1.819767014D+05-1.405347931D+03 1.103412258D+01-4.104591050D-04 9.031277570D-08
-1.033057360D-11 4.780551830D-16                -1.323136863D+05-3.738386080D+01
BF4-               Gurvich,1996a pt1 p63 pt2 p40.
 2 tpis96 B   1.00F   4.00E   1.00    0.00    0.00 0   86.8051614    -1761265.998
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13795.643
 2.068485200D+05-2.463190805D+03 1.206414196D+01 1.102766923D-02-1.751720760D-05
 1.201346256D-08-3.150588626D-12                -2.010569206D+05-4.610826940D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13795.643
-4.373241710D+05-7.759289410D+02 1.358222575D+01-2.341024178D-04 5.196915940D-08
-5.982245780D-12 2.781163206D-16                -2.127251877D+05-4.953369700D+01
BH                 Bauschlicher,1990. Gurvich,1996a pt1 p28 pt2 p19.
 2 g12/99 B   1.00H   1.00    0.00    0.00    0.00 0   11.8189400     448727.204
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8639.104
 2.063082550D+04-3.682502520D+02 6.071337870D+00-8.728321070D-03 1.458566459D-05
-1.036840401D-08 2.779462579D-12                 5.460459920D+04-1.300392582D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8639.104
-1.098531663D+06-1.745890126D+02 8.442426810D+00-5.440196670D-03 2.718307052D-06
-4.839812210D-10 2.868523222D-14                 5.016735670D+04-2.971030686D+01
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Appendix D (*continued*)

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BHCL              Gurvich,1996a pt1 p81 pt2 p58.
 2 g 9/98 B   1.00H   1.00CL  1.00    0.00    0.00 0   47.2719400     141418.307
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10304.807
 4.763274910D+04-4.420016520D+02 3.975645880D+00 8.541698760D-03-1.377785182D-05
 1.131521587D-08-3.569659180D-12                 1.822278428D+04 3.028452399D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10304.807
 3.499991720D+05-2.238404757D+03 8.711106050D+00-1.088882906D-03 4.189301090D-07
-6.568711260D-11 3.620067600D-15                 2.841240364D+04-2.589566225D+01
BHCL2             Gurvich,1996a pt1 p82 pt2 p60.
 2 tpis96 B   1.00H   1.00CL  2.00    0.00    0.00 0   82.7249400    -251883.529
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11745.632
 4.419914810D+04-2.384739577D+02 1.356682235D+00 2.517866897D-02-3.632910400D-05
 2.644335581D-08-7.625044110D-12                -3.003877914D+04 1.787024616D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11745.632
 4.110996060D+05-2.858027441D+03 1.179547506D+01-6.322817970D-04 1.269551549D-07
-1.352862344D-11 5.921653510D-16                -1.617288760D+04-4.217900972D+01
BHF               Gurvich,1996a pt1 p68 pt2 p45.
 2 g 9/98 B   1.00H   1.00F   1.00    0.00    0.00 0   30.8173432     -76012.343
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10042.057
-4.908362260D+04 9.610760210D+02-2.919850316D+00 2.149156633D-02-2.595677863D-05
 1.693492714D-08-4.553648840D-12                -1.466925195D+04 4.160709310D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10042.057
 1.184821300D+06-4.677435180D+03 1.067328148D+01-1.606366598D-03 3.704534700D-07
-3.797882750D-11 1.432441145D-15                 1.802640937D+04-4.285931170D+01
BHFCL             Gurvich,1996a pt1 p90 pt2 p69.
 2 tpis96 B   1.00H   1.00F   1.00CL  1.00    0.00 0   66.2703432    -483036.620
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11414.539
 5.761169720D+02 3.042156250D+02-9.808900360D-01 2.803843648D-02-3.676734020D-05
 2.499824138D-08-6.873421640D-12                -6.050207390D+04 3.132842092D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11414.539
 4.390778920D+05-3.137181709D+03 1.200286161D+01-7.153669340D-04 1.453878608D-07
-1.565197070D-11 6.910075060D-16                -4.232368340D+04-4.466542881D+01
BHF2              Gurvich,1996a pt1 p69 pt2 p47.
 2 tpis96 B   1.00H   1.00F   2.00    0.00    0.00 0   49.8157464     -739613.811
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10659.347
-8.353540280D+04 1.616659766D+03-8.161405670D+00 4.153786790D-02-4.921063280D-05
 3.054165306D-08-7.786813980D-12                -9.748065460D+04 7.038630750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10659.347
 4.660876960D+05-3.728100490D+03 1.244152658D+01-8.906843190D-04 1.841732568D-07
-2.010774349D-11 8.979196590D-16                -6.978142930D+04-5.103218040D+01
BH2               Jacox,1994.  Kolbuszewski,1996. Gurvich,1996a p32.
 2 g 2/00 B   1.00H   2.00    0.00    0.00    0.00 0   12.8268800     328909.059
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10023.559
 2.812557296D+04-3.000083489D+02 4.824221000D+00-2.186429819D-04 1.485457398D-06
 3.893739680D-10-6.331629390D-13                 3.991988420D+04-5.042682850D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10023.559
 1.360117365D+06-4.917704490D+03 9.758971030D+00-7.415870640D-04 1.269760019D-07
-1.187742442D-11 4.682552510D-16                 6.890292660D+04-4.190490120D+01
BH2CL             Gurvich,1996a pt1 p82 pt2 p59.
 2 tpis96 B   1.00H   2.00CL  1.00    0.00    0.00 0   48.2798800     -80845.754
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10426.902
 1.646638117D+04 1.277320942D+02 1.300268921D-01 1.938143193D-02-2.316389616D-05
 1.607896164D-08-4.668337650D-12                -1.112112215D+04 2.308500112D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10426.902
 1.427215437D+06-6.265564340D+03 1.382183005D+01-1.313843556D-03 2.587131606D-07
-2.713845270D-11 1.172827257D-15                 2.639387516D+04-6.399725308D+01
BH2F              Gurvich,1996a pt1 p69 pt2 p46.
 2 tpis96 B   1.00H   2.00F   1.00    0.00    0.00 0   31.8252832     -323956.732
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10137.922
-8.837920440D+04 1.705285929D+03-8.061246130D+00 3.643188680D-02-4.152482550D-05
 2.620135756D-08-6.930886410D-12                -4.787273410D+04 6.862087670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10137.922
 1.435082111D+06-6.625320170D+03 1.409165008D+01-1.422469060D-03 2.828724718D-07
-2.992498948D-11 1.302618926D-15                -7.937192670D+02-6.801356400D+01
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Appendix D (*continued*)

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BH3               Allendorf,1997. Jacox,1998 p212. Martin,1992.
 2 g 1/00 B   1.00H   3.00    0.00    0.00    0.00 0   13.8348200     104746.599
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10059.699
-6.619635070D+04 1.262658391D+03-4.654355900D+00 2.461795131D-02-2.501537437D-05
 1.562330756D-08-4.323949480D-12                 5.667587980D+03 4.666504620D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10059.699
 1.855778950D+06-8.002492370D+03 1.505692199D+01-1.790456689D-03 3.612511100D-07
-3.866035910D-11 1.698508879D-15                 5.967537070D+04-7.994046160D+01
BH3NH3            Gurvich,1996a pt1 p106 pt2 p84.
 2 tpis96 B   1.00H   6.00N   1.00    0.00    0.00 0   30.8653400    -115000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12681.530
-1.811063598D+05 3.010341543D+03-1.524271135D+01 6.215637750D-02-5.959881850D-05
 3.267429360D-08-7.751243090D-12                -2.934278877D+04 1.087399608D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12681.530
 4.354925960D+06-1.824235232D+04 3.162999830D+01-3.208243610D-03 5.885075450D-07
-5.808535530D-11 2.382578600D-15                 9.438118030D+04-1.897865799D+02
BH4               Radical. Saxon,1993. Yu,1998.
 2 g 5/00 B   1.00H   4.00    0.00    0.00    0.00 0   14.8427600     255210.477
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10770.877
 2.734274578D+04-8.473619380D+01 1.551871695D+00 1.439765491D-02-6.111152360D-06
-1.324417559D-10 5.133008150D-13                 3.022048074D+04 1.250358328D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10770.877
 1.354714146D+06-7.870762750D+03 1.826170610D+01-1.948275329D-03 4.072706890D-07
-4.482710900D-11 2.014115885D-15                 7.470249490D+04-9.686086890D+01
BH5               Schreiner,1994.
 2 g 8/00 B   1.00H   5.00    0.00    0.00    0.00 0   15.8507000      92933.658
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12572.458
-5.603075360D+04 1.457641959D+03-8.245037630D+00 4.817478230D-02-5.535104700D-05
 3.578299590D-08-9.717757500D-12                 3.424238930D+03 6.695881520D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12572.458
 2.472199159D+06-1.110339842D+04 2.243395706D+01-2.121632568D-03 4.038994240D-07
-4.121910490D-11 1.741706383D-15                 7.561744630D+04-1.243306259D+02
BI                Gurvich,1996a pt1 p94 pt2 p73.
 2 g 9/98 B   1.00I   1.00    0.00    0.00    0.00 0  137.7154700     325987.502
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9142.202
 3.517449530D+04-5.445819300D+02 6.027511010D+00-2.387237926D-03 2.244796277D-06
-1.110001347D-09 2.280204403D-13                 4.071910130D+04-7.288049840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9142.202
 2.132872626D+06-6.283684960D+03 1.123964343D+01-3.258856750D-03 7.064282150D-07
-4.230068930D-11-4.208078470D-16                 7.797634810D+04-4.664042610D+01
BI2               Gurvich,1996a pt1 p95 pt2 p74.
 2 g 9/98 B   1.00I   2.00    0.00    0.00    0.00 0  264.6199400     238096.324
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12688.424
 6.640975900D+04-1.044411994D+03 9.734197240D+00-3.952557540D-03 3.165567780D-06
-1.273764644D-09 1.879968132D-13                 3.205750890D+04-2.012407058D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12688.424
-3.924022230D+05 4.422902350D+02 7.129623580D+00-5.619634060D-04 3.180760520D-07
-5.537079720D-11 3.183959700D-15                 2.291972638D+04-3.201793240D+00
BI3               Gurvich,1996a pt1 p96 pt2 p75.
 2 tpis96 B   1.00I   3.00    0.00    0.00    0.00 0  391.5244100      21400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16933.072
 6.243114890D+04-1.002408628D+03 1.106650075D+01 1.609588058D-03-5.147250250D-06
 4.732514020D-09-1.512999796D-12                 5.160348150D+03-2.420687643D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16933.072
-1.506176506D+05-8.167210610D+01 1.005937867D+01-2.319396215D-05 5.019966730D-09
-5.654349630D-13 2.580651348D-17                -4.261687910D+02-1.617962779D+01
BN                Gurvich,1996a pt1 p104 pt2 p83.
 2 g 9/98 B   1.00N   1.00    0.00    0.00    0.00 0   24.8177000     574726.408
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8961.108
-4.569707580D+04 6.704286070D+02 3.615089080D-02 7.339487510D-03-4.969033490D-06
 1.229031380D-09 6.340281520D-14                 6.485465080D+04 2.539869896D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8961.108
-2.276932705D+05-1.025649298D+02 4.414586810D+00 2.561670989D-04-1.612994942D-08
-6.526052930D-13 5.749466120D-17                 6.784465130D+04-6.778568656D-01
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BO                Gurvich,1996a pt1 p10 pt2 p8.
 3 g 9/98 B   1.00O   1.00    0.00    0.00    0.00 0   26.8104000      20406.404
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.104
-1.166216822D+04 9.217579390D+01 3.655498490D+00-3.118542920D-03 9.008329830D-06
-8.017789990D-09 2.472952292D-12                 8.738284780D+02 4.482847390D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.104
 1.788600589D+04-6.309019630D+02 4.574528400D+00 1.988001643D-04-9.702963480D-08
 1.870854291D-11-1.030218131D-15                 4.841311090D+03-3.398890580D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.104
-1.592699514D+08 1.210955629D+05-3.136823502D+01 5.110037760D-03-3.461020740D-07
 1.148046833D-11-1.504899225D-16                -9.345065760D+05 3.026123907D+02
BO-               Gurvich,1996a pt1 p13 pt2 p10.
 2 g 9/98 B   1.00O   1.00E   1.00    0.00    0.00 0   26.8109486    -277791.076
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.024
-8.242023210D+04 9.203636900D+02-2.302659981D-01 6.229904120D-03-3.157624391D-06
 1.184578107D-10 2.819228693D-13                -3.911141220D+04 2.599226838D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.024
 2.122804369D+05-1.262124688D+03 5.383167310D+00-3.181049100D-04 7.288988250D-08
-8.141708920D-12 3.715364390D-16                -2.706892261D+04-9.773753670D+00
BOCL              Gurvich,1996a pt1 p79 pt2 p55.
 2 tpis96 B   1.00O   1.00CL  1.00    0.00    0.00 0   62.2634000    -318536.695
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10607.913
 7.052380640D+04-1.315301429D+03 1.130087727D+01-1.207112050D-02 1.880516131D-05
-1.373823975D-08 3.854890160D-12                -3.355399100D+04-3.698462517D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10607.913
 1.557148487D+05-1.446254968D+03 8.509448050D+00-3.859007380D-04 8.262268820D-08
-9.261027460D-12 4.219998010D-16                -3.203589040D+04-2.372713292D+01
BOCL2             Gurvich,1996a pt1 p79 pt2 p56.
 2 tpis96 B   1.00O   1.00CL  2.00    0.00    0.00 0   97.7164000    -361565.512
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13169.650
 7.322667360D+03-2.027726965D+02 4.161924090D+00 1.733309456D-02-2.263908718D-05
 1.452275190D-08-3.719593120D-12                -4.414441880D+04 6.520424110D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13169.650
-2.297527041D+05-6.194567930D+02 1.046075518D+01-1.841620739D-04 4.071215430D-08
-4.672246550D-12 2.167237536D-16                -4.371538420D+04-2.743570215D+01
BOF               Gurvich,1996a pt1 p65 pt2 p42.
 2 tpis96 B   1.00O   1.00F   1.00    0.00    0.00 0   45.8088032    -592978.311
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9988.295
 7.226802650D+04-1.131386630D+03 8.816054520D+00-4.627694570D-03 7.801299580D-06
-5.681205840D-09 1.534732094D-12                -6.711116010D+04-2.547957229D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9988.295
 1.937020297D+05-1.739112297D+03 8.695650860D+00-4.518895570D-04 9.591019080D-08
-1.067806769D-11 4.840007660D-16                -6.330152390D+04-2.702458617D+01
BOF2              Gurvich,1996a pt1 p66 pt2 p43.
 2 tpis96 B   1.00O   1.00F   2.00    0.00    0.00 0   64.8072064    -832767.700
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11611.458
 7.227794130D+03 2.148783624D+01 1.157840301D+00 2.250585296D-02-2.610731536D-05
 1.508824929D-08-3.518364850D-12                -1.013995733D+05 2.010127136D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11611.458
-2.205028861D+05-1.254238690D+03 1.092551380D+01-3.680144000D-04 8.107164940D-08
-9.281275060D-12 4.297549300D-16                -9.680447580D+04-3.482853330D+01
BOH               Gurvich,1996a pt1 p41 pt2 p24.
 2 tpis96 B   1.00O   1.00H   1.00    0.00    0.00 0   27.8183400      -6756.578
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10031.524
-7.521410270D+04 1.391444703D+03-5.630330180D+00 2.966358811D-02-3.830835180D-05
 2.550606424D-08-6.795857210D-12                -8.341300280D+03 5.517690040D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10031.524
 8.447498570D+05-3.016982887D+03 8.083864700D+00-1.609855388D-04-2.191830959D-09
 3.127133119D-12-2.376665451D-16                 1.647698495D+04-2.603227947D+01
BO2               Gurvich,1996a pt1 p14 pt2 p11.
 2 g10/97 B   1.00O   2.00    0.00    0.00    0.00 0   42.8098000    -309121.947
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10772.157
-4.141090640D+04 7.198854610D+02-1.477629435D+00 2.277415194D-02-2.786326934D-05
 1.718462069D-08-4.278991440D-12                -4.177657690D+04 3.258458010D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10772.157
-3.834452340D+04-9.563261140D+02 8.200962780D+00-2.062130802D-04 9.872288990D-09
 8.158366760D-12-7.527519660D-16                -3.423564020D+04-2.224772278D+01
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BO2-              Gurvich,1996a pt1 p16 pt2 p13.
 2 tpis96 B   1.00O   2.00E   1.00     0.00     0.00 0   42.8103486     -714493.991
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9597.541
 5.324279690D+04-7.326313030D+02 5.902470000D+00 2.437465200D-03-4.878803950D-07
-8.475724760D-10 4.080781180D-13                -8.344293680D+04-1.053931911D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9597.541
 1.199226372D+05-1.715766982D+03 8.701038220D+00-4.601242120D-04 9.867011870D-08
-1.107288516D-11 5.050183240D-16                -7.825789690D+04-2.839356505D+01
B(OH)2            Gurvich,1996a pt1 p46 pt2 p28.
 2 g 9/98 B   1.00O   2.00H   2.00     0.00     0.00 0   44.8256800     -425243.642
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11971.658
 1.491659222D+03 3.648184840D+02-2.906006389D+00 4.136834460D-02-5.782584220D-05
 4.069783560D-08-1.126499791D-11                -5.375483660D+04 3.888535180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11971.658
 1.557023406D+06-5.784710760D+03 1.487391235D+01-1.821804765D-04-3.803541640D-08
 1.030332746D-11-6.685889830D-16                -1.806810301D+04-6.590268900D+01
BS                Gurvich,1996a pt1 p97 pt2 p76.
 2 g10/98 B   1.00S   1.00     0.00     0.00     0.00 0   42.8760000      273519.405
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8724.105
-3.839490100D+04 6.989417490D+02-1.213980460D+00 1.396391264D-02-1.689881284D-05
 1.038889985D-08-2.582063989D-12                2.865685472D+04 3.154819945D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8724.105
 1.358760165D+06-4.364035960D+03 9.034307590D+00-2.114548699D-03 4.189275310D-07
-1.354787322D-11-1.360684605D-15                5.913065450D+04-3.336696868D+01
BS2               Gurvich,1996a pt1 p99 pt2 p77.
 2 g 9/98 B   1.00S   2.00     0.00     0.00     0.00 0   74.9410000      63867.460
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13559.560
 1.820264374D+04-5.150671890D+02 8.547515000D+00-1.626155268D-03 1.866387194D-06
-1.277165468D-09 3.681980690D-13                8.186839750D+03-1.778384854D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13559.560
 5.120402510D+05-1.938581076D+03 9.814873460D+00-1.339731606D-03 3.754301160D-07
-4.400383780D-11 1.887662968D-15                1.736535000D+04-2.757546712D+01
B2                Gurvich,1996a pt1 p8 pt2 p7.
 2 g 9/98 B   2.00     0.00     0.00     0.00     0.00 0   21.6220000      857370.506
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8805.106
-1.516418096D+05 2.630168946D+03-1.381358321D+01 5.216225190D-02-6.930494740D-05
 4.469410390D-08-1.128496456D-11                8.995251050D+04 9.813118490D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8805.106
 1.094594495D+06-2.602735739D+03 6.909456210D+00-6.405949890D-04 1.951732355D-07
-2.555902119D-11 1.053557323D-15                1.187807611D+05-1.949045025D+01
B2C               Gurvich,1996a pt1 p110 pt2 p88.
 2 g 9/98 B   2.00C   1.00     0.00     0.00     0.00 0   33.6327000      800432.614
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11723.114
-4.166519870D+04 5.797779520D+02 1.411017091D+00 1.174705713D-02-1.066474425D-05
 4.717232620D-09-7.970013260D-13                9.196874200D+04 1.769254387D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11723.114
 1.159241019D+06-4.567798810D+03 1.228672097D+01-2.500830701D-03 6.409979850D-07
-6.932935770D-11 2.672933741D-15                1.222442137D+05-5.199066186D+01
B2CL4             Gurvich,1996a pt1 p77 pt2 p54.
 2 g10/97 B   2.00CL  4.00     0.00     0.00     0.00 0  163.4340000     -490000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21588.132
 4.285555130D+04-7.280748810D+02 9.315763670D+00 2.331629623D-02-3.511247610D-05
 2.464057658D-08-6.735479960D-12               -5.819023240D+04-1.622083878D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21588.132
-6.427987030D+05 5.078562990D+02 1.486725022D+01 2.026983515D-06 6.272718810D-09
-1.218822573D-12 7.241208410D-17               -6.820066000D+04-4.139110669D+01
B2F4              Gurvich,1996a pt1 p64 pt2 p41.
 2 g10/97 B   2.00F   4.00     0.00     0.00     0.00 0   97.6156128    -1438000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17680.793
-5.971695640D+04 8.189425440D+02-6.437671290D-01 3.858966070D-02-4.313053190D-05
 2.404463223D-08-5.393559350D-12               -1.790041225D+05 3.552179970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17680.793
 3.855865890D+04-2.928842655D+03 1.792063736D+01-9.523998270D-04 1.614708845D-07
-1.428613504D-11 5.218739670D-16               -1.613051924D+05-7.184803250D+01
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Appendix D (*continued*)

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B2H                Adams,1989. Yu,1998.
 2 g 7/00 B   2.00H   1.00    0.00    0.00    0.00 0   22.6299400     796262.497
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10115.597
 8.775579740D+04-1.343931564D+03 9.832099150D+00-5.607137750D-03 5.730651050D-06
-2.266436197D-09 1.972352080D-13                 1.009908698D+05-3.282461480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10115.597
 6.175545750D+05-2.627897466D+03 9.084905070D+00-5.389418330D-04 1.050714700D-07
-1.092459556D-11 4.684854660D-16                 1.099537555D+05-3.164029910D+01
B2H2               Curtiss,1989a. Yu,1998.
 2 g 7/00 B   2.00H   2.00    0.00    0.00    0.00 0   23.6378800     454677.939
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10573.239
 1.421617322D+05-2.138011262D+03 1.317732399D+01-8.942658070D-03 1.127804935D-05
-5.787886200D-09 1.000813871D-12                 6.372319250D+04-5.346982740D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10573.239
 1.240614592D+06-5.368965020D+03 1.379292454D+01-1.136749748D-03 2.245617156D-07
-2.361530467D-11 1.022604572D-15                 8.506511490D+04-6.435461300D+01
B2H3               Adams,1989. Yu,1998.
 2 g 6/00 B   2.00H   3.00    0.00    0.00    0.00 0   24.6458200     351072.721
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11938.621
 9.425147160D+04-1.075866284D+03 6.383999390D+00 1.167858327D-02-1.429661252D-05
 1.128776882D-08-3.681325060D-12                 4.635335080D+04-1.400002845D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11938.621
 1.771506902D+06-7.872260930D+03 1.789447015D+01-1.709304785D-03 3.409575430D-07
-3.614543680D-11 1.575671409D-15                 8.737711890D+04-9.054629460D+01
B2H3,db            2-Bridges. Adams,1989. Yu,1998.
 2 g 7/00 B   2.00H   3.00    0.00    0.00    0.00 0   24.6458200     353408.227
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11911.227
 6.064014840D+04-7.524466330D+02 5.584483840D+00 1.080468494D-02-8.649032810D-06
 4.748333310D-09-1.309096028D-12                 4.491792300D+04-8.873686820D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11911.227
 1.497731017D+06-7.219314140D+03 1.750463766D+01-1.579698800D-03 3.164103470D-07
-3.367225150D-11 1.472919654D-15                 8.324349670D+04-8.779549260D+01
B2H4               1-Bridge. Ruscic,1989b. Curtiss,1989b.
 2 g 8/00 B   2.00H   4.00    0.00    0.00    0.00 0   25.6537600     211162.059
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12339.859
 4.000132300D+04-3.071548876D+02 1.763071673D+00 2.646361882D-02-3.066168202D-05
 2.163781936D-08-6.491835410D-12                 2.581033714D+04 1.015267130D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12339.859
 2.292078842D+06-1.059832517D+04 2.268612155D+01-2.363586598D-03 4.762173070D-07
-5.090100400D-11 2.233911590D-15                 8.638591980D+04-1.246794566D+02
B2H4,db            2-Bridges.Ruscic,1989b. Curtiss,1989b.
 2 g 7/00 B   2.00H   4.00    0.00    0.00    0.00 0   25.6537600     209932.448
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11528.648
-1.781496923D+04 5.716048040D+02-2.763085348D+00 3.125348696D-02-2.709524346D-05
 1.341728634D-08-3.004352798D-12                 2.158138307D+04 3.675872940D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11528.648
 1.886854256D+06-1.010045614D+04 2.247110812D+01-2.319968667D-03 4.731879960D-07
-5.110673030D-11 2.262693782D-15                 8.233487000D+04-1.237455797D+02
B2H5               1-Bridge. Ruscic,1989a. Trachtman,1989.
 2 g 5/00 B   2.00H   5.00    0.00    0.00    0.00 0   26.6617000     254783.889
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12220.789
 3.830965450D+04-4.066148050D+01-1.422523787D+00 3.674595270D-02-3.851989710D-05
 2.444494440D-08-6.821722940D-12                 3.008956452D+04 2.802425895D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12220.789
 2.696691012D+06-1.320019835D+04 2.735260413D+01-2.961879012D-03 5.984999430D-07
-6.413748550D-11 2.821187823D-15                 1.064524901D+05-1.559654379D+02
B2H5,db            2-Bridges. Ruscic,1989a. Trachtman,1989.
 2 g 5/00 B   2.00H   5.00    0.00    0.00    0.00 0   26.6617000     275150.616
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11667.516
 1.424446027D+04 4.204558200D+02-3.700451250D+00 3.672053100D-02-3.193503730D-05
 1.695013434D-08-4.257038140D-12                 3.046684683D+04 4.245495820D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11667.516
 2.571729448D+06-1.356829858D+04 2.781376038D+01-3.192365030D-03 6.561165260D-07
-7.127333940D-11 3.169492650D-15                 1.106370527D+05-1.597214457D+02
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B2H6              Hf:Gurvich,1996a pt1 p37. Yu,1998. Duncan,1985.
 2 g 5/00 B   2.00H   6.00    0.00    0.00    0.00 0   27.6696400      36600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11932.313
-1.052844558D+04 1.041795556D+03-8.960518860D+00 5.492480880D-02-5.305197050D-05
 3.011904756D-08-7.688768300D-12                -9.259374350D+02 6.812592430D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11932.313
 2.835765414D+06-1.567600163D+04 3.226122330D+01-3.738609730D-03 7.718806460D-07
-8.414454540D-11 3.752223380D-15                 9.358378550D+04-1.920223395D+02
B2O               Gurvich,1996a pt1 p19 pt2 p14.
 2 g 9/98 B   2.00O   1.00    0.00    0.00    0.00 0   37.6214000     192798.018
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11783.018
-5.699546760D+04 1.018000465D+03-2.636481947D+00 2.746009279D-02-3.632432720D-05
 2.406890217D-08-6.384129720D-12                 1.703874394D+04 3.855346110D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11783.018
-1.628723220D+05-3.876289810D+02 7.787723520D+00-1.146822108D-04 2.528097612D-08
-2.893783941D-12 1.339210475D-16                 2.263035354D+04-1.908513011D+01
B2O2              Gurvich,1996a pt1 p19 pt2 p15.
 2 tpis96 B   2.00O   2.00    0.00    0.00    0.00 0   53.6208000    -457711.486
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13396.618
 8.174391690D+04-1.732702797D+03 1.605560926D+01-2.160057288D-02 3.566854570D-05
-2.660198794D-08 7.531833240D-12                -4.899632900D+04-6.172702390D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13396.618
 4.605789660D+05-2.990079203D+03 1.256764079D+01-7.850974950D-04 1.672537624D-07
-1.867694780D-11 8.486190670D-16                -4.015748150D+04-4.874413710D+01
B2O3              Gurvich,1996a pt1 p25 pt2 p18.
 2 tpis96 B   2.00O   3.00    0.00    0.00    0.00 0   69.6202000    -835382.271
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14418.729
 7.379611910D+04-1.263620592D+03 1.072681512D+01 3.841383720D-04 5.976058380D-06
-6.552891350D-09 2.123951064D-12                -9.628183140D+04-3.088078011D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14418.729
 3.905035300D+05-3.691348210D+03 1.555502598D+01-9.707645510D-04 2.068887872D-07
-2.310858356D-11 1.050136734D-15                -8.263054410D+04-6.390863440D+01
B2(OH)4           Gurvich,1996a pt1 p52 pt2 p33.
 2 g 9/98 B   2.00O   4.00H   4.00    0.00    0.00 0   89.6513600   -1254987.531
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19443.069
-1.728717249D+04 8.495913480D+02-8.715959570D+00 9.362362610D-02-1.278784165D-04
 8.813671160D-08-2.400605571D-11                -1.564337133D+05 7.120169310D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19443.069
 2.983925656D+06-1.207469577D+04 3.162610570D+01-5.163682440D-04-4.232093970D-08
 1.671977280D-11-1.156366726D-15                -8.280976970D+04-1.653010498D+02
B2S               Gurvich,1996a pt1 p100, pt2 p78.
 2 g 9/98 B   2.00S   1.00    0.00    0.00    0.00 0   53.6870000     622260.705
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13182.705
 6.638609300D+04-9.201185690D+02 8.699831340D+00 7.645589010D-04-3.709026030D-06
 3.642373980D-09-1.197766071D-12                 7.770375800D+04-2.251712444D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13182.705
-1.211501483D+05-6.473398450D+01 7.546825610D+00-1.820541450D-05 3.923951170D-09
-4.403862380D-13 2.003651718D-17                 7.258531870D+04-1.394971229D+01
B2S2              Gurvich,1996a pt1 p100 pt2 p79.
 2 tpis96 B   2.00S   2.00    0.00    0.00    0.00 0   85.7520000     138317.112
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14569.112
-7.061549970D+04 7.182944780D+02 1.919797788D+00 2.036407461D-02-2.309813846D-05
 1.311616725D-08-2.996394781D-12                 1.100829019D+04 1.855402586D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14569.112
-1.641535014D+05-7.742865640D+02 1.107731737D+01-2.313278554D-04 5.125614290D-08
-5.894081230D-12 2.738673834D-16                 1.733003515D+04-3.359766998D+01
B2S3              Gurvich,1996a pt1 p102 pt2 p81.
 2 tpis96 B   2.00S   3.00    0.00    0.00    0.00 0  117.8170000     17754.057
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19938.057
-3.431268500D+04 5.587615370D+02 3.414077410D+00 2.398333891D-02-2.841617637D-05
 1.690005199D-08-4.060070710D-12                -3.027690575D+03 1.846767864D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19938.057
-1.905855086D+05-9.348342480D+02 1.369333613D+01-2.766647250D-04 6.110155800D-08
-7.008048570D-12 3.249524620D-16                 2.906433760D+03-3.946870479D+01
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B3H7,C2v          C2v symmetry. Stanton,1989b.
 2 g 8/00 B   3.00H   7.00    0.00    0.00    0.00 0   39.4885800     176019.139
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14818.439
 1.086009469D+05-7.921536800D+02-9.577368040D-01 5.656119290D-02-6.405034500D-05
 4.281322960D-08-1.227580455D-11                 2.430638819D+04 2.102582666D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14818.439
 3.598592140D+06-1.863701968D+04 3.993998830D+01-4.275410160D-03 8.705358820D-07
-9.385105020D-11 4.147865310D-15                 1.272154092D+05-2.379769856D+02
B3H7,Cs           Cs symmetry. Stanton,1989b.
 2 g 8/00 B   3.00H   7.00    0.00    0.00    0.00 0   39.4885800     159318.322
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14083.322
 5.298169330D+04 4.071745370D+02-9.635730530D+00 7.944312000D-02-9.306456820D-05
 6.105147350D-08-1.685927691D-11                 1.707069083D+04 6.873966560D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14083.322
 3.281576450D+06-1.811096595D+04 3.963832460D+01-4.178424110D-03 8.526829060D-07
-9.209600240D-11 4.076496770D-15                 1.213622564D+05-2.357090217D+02
B3H9              Hf:McKee,1990. Stanton,1989a.
 2 g 7/00 B   3.00H   9.00    0.00    0.00    0.00 0   41.5044600     138908.800
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17329.935
 8.483214900D+04-5.206163040D+02-4.665701210D-01 5.346983860D-02-4.155796820D-05
 1.944135439D-08-4.541227350D-12                 1.805101100D+04 2.110804198D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17329.935
 3.863999500D+06-2.229433407D+04 4.875046150D+01-5.418449260D-03 1.125767651D-06
-1.233226406D-10 5.520348180D-15                 1.422187123D+05-2.958240102D+02
B3N3H6            Borazole.  Gurvich,1996a pt1 p107 pt2 p85.
 2 tpis96 B   3.00N   3.00H   6.00    0.00    0.00 0   80.5007400    -512000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16221.348
-1.552621082D+05 4.010211270D+03-3.382491300D+01 1.624575582D-01-2.065528647D-04
 1.368862991D-07-3.673470900D-11                -8.051253400D+04 1.995000751D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16221.348
 3.739245170D+06-1.941238951D+04 4.445070030D+01-3.210308050D-03 5.717465420D-07
-5.486692140D-11 2.191943197D-15                 4.758426160D+04-2.641156625D+02
B3O3CL3           Gurvich,1996a pt1 p80 pt2 p57.
 2 tpis96 B   3.00O   3.00CL  3.00    0.00    0.00 0  186.7902000   -1635982.041
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24451.781
-4.284452800D+04 1.005623966D+03-4.556519630D+00 8.117967140D-02-1.038385803D-04
 6.621422330D-08-1.695748504D-11                -2.040907277D+05 5.466113803D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24451.781
-7.414059810D+05-2.527447455D+03 2.687263667D+01-7.463389360D-04 1.646334110D-07
-1.886231553D-11 8.737926310D-16                -1.923509858D+05-1.185636255D+02
B3O3FCL2          Gurvich,1996a pt1 p89 pt2 p68.
 2 tpis96 B   3.00O   3.00F   1.00CL  2.00    0.00 0  170.3356032   -1883807.681
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23448.139
-3.719120070D+04 8.673745890D+02-4.095778460D+00 7.815563970D-02-9.767035170D-05
 6.097610090D-08-1.532880319D-11                -2.331383552D+05 5.198088158D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23448.139
-7.162360830D+05-2.851210308D+03 2.710953133D+01-8.400919640D-04 1.852318684D-07
-2.121694694D-11 9.827291560D-16                -2.202729252D+05-1.210679365D+02
B3O3F2CL          Gurvich,1996a pt1 p89 pt2 p67.
 2 tpis96 B   3.00O   3.00F   2.00CL  1.00    0.00 0  153.8810064   -2132816.827
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22260.991
-5.277015540D+04 1.104904696D+03-5.854181050D+00 7.953943100D-02-9.592660770D-05
 5.799856310D-08-1.416698348D-11                -2.640400115D+05 6.071247222D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22260.991
-6.810787490D+05-3.370009020D+03 2.748953579D+01-9.905442560D-04 2.182908440D-07
-2.499573480D-11 1.157532106D-15                -2.472114785D+05-1.261501548D+02
B3O3F3            Gurvich,1996a pt1 p67 pt2 p44.
 2 tpis96 B   3.00O   3.00F   3.00    0.00    0.00 0  137.4264096   -2382699.078
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21200.738
-7.251549780D+04 1.400996228D+03-7.906716200D+00 8.217161850D-02-9.633152660D-05
 5.668194260D-08-1.349024305D-11                -2.953461728D+05 7.001536830D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21200.738
-6.629822910D+05-3.784946870D+03 2.779526578D+01-1.112096232D-03 2.450806704D-07
-2.806484980D-11 1.299750466D-15                -2.748865475D+05-1.315605015D+02
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B4H4              Yu,1998. Mach,1994.
 2 g 8/00 B   4.00H   4.00     0.00     0.00     0.00 0   47.2757600      326190.400
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14936.602
 2.171791579D+05-2.598282557D+03 9.845440610D+00 3.026309140D-02-4.128334160D-05
 3.089368344D-08-9.353384260D-12                 5.079143480D+04-3.770757210D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14936.602
 1.937200886D+06-1.078185932D+04 2.879625241D+01-2.401547707D-03 4.837756780D-07
-5.170490230D-11 2.269138182D-15                 9.836595390D+04-1.561814117D+02
B4H10             Wagman,1982 p123. McKee,1990. Dain,1981.
 2 g 5/00 B   4.00H  10.00     0.00     0.00     0.00 0   53.3234000      66100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15485.574
-3.296604820D+04 2.440532922D+03-2.685332563D+01 1.406499347D-01-1.586710574D-04
 9.874594130D-08-2.601426018D-11                -3.091924018D+03 1.589905532D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15485.574
 4.030474130D+06-2.560629762D+04 5.687233660D+01-6.178567860D-03 1.280621032D-06
-1.400254585D-10 6.258866560D-15                 1.506009087D+05-3.520714200D+02
B4H12             Shen,1993. Yu,1998.
 2 g 5/00 B   4.00H  12.00     0.00     0.00     0.00 0   55.3392800      188236.114
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21748.714
 7.152170300D+04-1.590351575D+02-4.719771660D+00 8.811228900D-02-8.604946880D-05
 5.123535510D-08-1.379865250D-11                 2.194186547D+04 4.187897400D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21748.714
 6.158360800D+06-3.202086730D+04 6.660443600D+01-7.406369280D-03 1.512993908D-06
-1.635619071D-10 7.245385140D-15                 2.054586275D+05-4.142106860D+02
B5H9              Hf:Chase,1998 p303 3/65.McKee,1990.Beaudet,1988.Yu,1998.
 2 g 6/00 B   5.00H   9.00     0.00     0.00     0.00 0   63.1264600      73220.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16052.677
 8.998473720D+04 1.042533357D+02-1.195549834D+01 1.007310686D-01-9.866680210D-05
 5.295535180D-08-1.232119583D-11                 8.374341780D+03 7.663090480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16052.677
 3.169017620D+06-2.282503203D+04 5.512008980D+01-5.563411420D-03 1.157837073D-06
-1.270332301D-10 5.694262030D-15                 1.334452571D+05-3.371060460D+02
Ba                Gurvich,1996. Moore,1971. Moore,1970a. Gordon,1999.
 3 g10/97 BA  1.00     0.00     0.00     0.00     0.00 0  137.3270000      185000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 2.222563526D+03-3.407977850D+01 2.706751118D+00-6.382894490D-04 1.063003846D-06
-9.102624270D-10 3.148062219D-13                 2.166549702D+04 5.102545880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-1.926579228D+07 6.006501040D+04-6.633964130D+01 3.507565930D-02-7.807601830D-06
 8.085126800D-10-3.199486918D-14                -3.589663720D+05 5.007583400D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 3.483452070D+08-2.925558261D+05 9.774888490D+01-1.345477126D-02 9.567239790D-07
-3.380662310D-11 4.727390540D-16                 2.250335260D+06-7.968444410D+02
Ba+               Moore,1971. Gordon,1999.
 3 g10/97 BA  1.00E  -1.00     0.00     0.00     0.00 0  137.3264514      694049.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-5.423167550D+04 6.744680780D+02-8.940272500D-01 8.796642950D-03-1.222812901D-05
 8.387953870D-09-2.037964358D-12                 7.941774640D+04 2.607063698D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 8.794971850D+06-1.951817883D+04 1.485542861D+01-9.404233500D-04-7.031257790D-07
 1.667412753D-10-1.070117310D-14                 2.146800732D+05-9.228264190D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-1.055569557D+08 4.530799570D+04-5.410673220D-01-7.531497600D-04 1.295568595D-07
-6.013388590D-12 8.846178515D-17                -3.000874708D+05 4.370610780D+01
BaBr              Gurvich,1996a pt1 p576 pt2 p437.
 2 tpis96 BA  1.00BR  1.00     0.00     0.00     0.00 0  217.2310000     -75324.677
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10200.123
-6.912557440D+02-6.245500160D+01 4.796677650D+00-6.838004940D-04 1.043947680D-06
-7.441224300D-10 2.172187003D-13                -1.011349165D+04 5.196454870D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10200.123
-1.056014042D+06 1.034740207D+03 6.735729380D+00-3.784026300D-03 1.952196896D-06
-3.347831880D-10 1.893189803D-14                -1.950233645D+04-5.069279640D+00
BaBr2             Gurvich,1996a pt1 p579 pt2 p439.
 2 tpis96 BA  1.00BR  2.00     0.00     0.00     0.00 0  297.1350000     -412514.741
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15485.759
-5.143374060D+03-3.870518460D+01 7.162446970D+00-3.696715310D-04 4.689715270D-07
-3.107902475D-10 8.363582050D-14                -5.153318260D+04 9.741407000D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15485.759
-8.928251210D+03-7.536558890D-01 7.000658210D+00-2.949821710D-07 7.092392110D-11
-8.670038100D-15 4.221742310D-19                -5.172669490D+04 1.910185706D+00
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BaCL              Gurvich,1996a pt1 p570 pt2 p433.
 2 tpis96 BA  1.00CL  1.00     0.00     0.00     0.00 0  172.7800000     -136290.881
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9877.119
-2.661946867D+03-7.724996340D+01 4.746106050D+00-3.523548880D-04 3.999198350D-07
-1.936413749D-10 4.124048530D-14                 -1.736328141D+04 3.904455084D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9877.119
-1.075410089D+06 1.209303069D+03 6.272558600D+00-3.288110310D-03 1.717751087D-06
-2.910607065D-10 1.632658438D-14                 -2.779173737D+04-3.574185216D+00
BaCL+             Gurvich,1996a pt1 p572 pt2 p434.
 2 g12/97 BA  1.00CL  1.00E  -1.00     0.00     0.00 0  172.7794514      348697.630
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9668.230
-8.951556690D+02-1.334692684D+02 4.935416120D+00-7.574054510D-04 8.355724000D-07
-4.685258510D-10 1.095343103D-13                  4.125155990D+04 1.896278378D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9668.230
-1.829198157D+04-2.931616688D+00 4.502280710D+00 3.671788490D-05 2.396147871D-09
 5.479458600D-14 1.174342316D-18                  4.055100150D+04 4.503765564D+00
BaCL2             Gurvich,1996a pt1 p575 pt2 p436.
 2 tpis96 BA  1.00CL  2.00     0.00     0.00     0.00 0  208.2330000     -499301.387
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14599.113
-1.157501999D+03-2.054518828D+02 7.837514050D+00-1.867700704D-03 2.335378734D-06
-1.531373341D-09 4.088525090D-13                 -6.115665280D+04-5.978149218D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14599.113
-2.216598768D+04-4.002483810D+00 7.003426740D+00-1.515820808D-06 3.611849210D-10
-4.386759060D-14 2.125803293D-18                 -6.219095270D+04-1.132439694D+00
BaF               Gurvich,1996a pt1 p562 pt2 p429.
 2 tpis96 BA  1.00F   1.00     0.00     0.00     0.00 0  156.3254032     -318993.788
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9342.112
 2.530317292D+04-4.716995100D+02 6.185036220D+00-3.366678800D-03 4.011834560D-06
-2.506578601D-09 6.477258160D-13                 -3.731872140D+04-6.220715380D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9342.112
 1.868380434D+06-7.071099600D+03 1.466959284D+01-6.995950200D-03 2.366313845D-06
-3.287734300D-10 1.647896238D-14                  3.571780680D+03-6.662390920D+01
BaF+              Gurvich,1996a pt1 p566 pt2 p430.
 2 g12/97 BA  1.00F   1.00E  -1.00     0.00     0.00 0  156.3248546      134063.214
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9201.714
 2.840719922D+04-4.863571820D+02 5.946058390D+00-2.429844077D-03 2.445346729D-06
-1.316757471D-09 2.974886320D-13                  1.730639076D+04-5.951206930D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9201.714
-4.054423670D+04-1.701997704D+01 4.513055340D+00 2.632753508D-05 2.612088236D-09
-9.502197930D-14 6.515176160D-18                  1.474486570D+04 2.783167711D+00
BaF2              Gurvich,1996a pt1 p569 pt2 p432.
 2 tpis96 BA  1.00F   2.00     0.00     0.00     0.00 0  175.3238064     -812003.483
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13437.017
 3.488395520D+04-7.648459560D+02 9.797750380D+00-5.756457510D-03 6.775603800D-06
-4.243614750D-09 1.093687692D-12                 -9.590356450D+04-2.082035292D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13437.017
-5.508633660D+04-1.691114228D+01 7.013564880D+00-5.731909770D-06 1.321203959D-09
-1.565528167D-13 7.444983020D-18                 -9.983529700D+04-4.389581490D+00
BaH               Gurvich,1996a pt1 p554 pt2 p423.
 2 tpis96 BA  1.00H   1.00     0.00     0.00     0.00 0  138.3349400      209535.105
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8731.105
-3.765268880D+04 6.986680120D+02-1.313524351D+00 1.460648882D-02-1.802974829D-05
 1.133031115D-08-2.865589059D-12                  2.097478889D+04 3.230802600D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8731.105
-6.755466570D+06 1.730700212D+04-1.136812458D+01 5.617744740D-03-3.180788850D-07
-1.052342502D-10 1.111101879D-14                 -8.954070380D+04 1.182377538D+02
BaI               Gurvich,1996a pt1 p581 pt2 p440.
 2 tpis96 BA  1.00I   1.00     0.00     0.00     0.00 0  264.2314700     -10237.675
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10397.125
-4.186285540D+03 1.033094613D+01 4.428900230D+00 3.026019976D-04-2.591429408D-07
 1.741605400D-10-3.370062760D-14                 -2.636169733D+03 8.201924680D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10397.125
-3.533859660D+06 7.394258000D+03 1.285151488D+00-2.303429302D-03 2.214839289D-06
-4.681096810D-10 3.011371472D-14                 -5.340229590D+04 3.710443870D+01
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Appendix D (*continued*)

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BaI2              Gurvich,1996a pt1 p584 pt2 p442.
 2 tpis96 BA  1.00I   2.00    0.00    0.00    0.00 0  391.1359400    -288439.965
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15790.435
-4.241592730D+03-1.862214382D+01 7.078556750D+00-1.793922821D-04 2.281437677D-07
-1.514647881D-10 4.081498360D-14                -3.670351490D+04 3.163138970D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15790.435
-6.048224800D+03-3.622729450D-01 7.000317450D+00-1.425793502D-07 3.433349420D-11
-4.201754980D-15 2.047703474D-19                -3.679650750D+04 3.615475320D+00
BaO               Gurvich,1996a pt1 p550 pt2 p419.
 3 tpis96 BA  1.00O   1.00    0.00    0.00    0.00 0  153.3264000    -117948.392
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9014.108
 3.764398500D+04-5.071555300D+02 5.392847280D+00-4.119324690D-04-6.527896620D-07
 9.430588420D-10-3.436603030D-13                -1.275552614D+04-3.752213760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9014.108
 1.318481698D+07-3.854253250D+04 4.686741610D+01-2.188646633D-02 5.335677450D-06
-5.152304300D-10 1.433083400D-14                 2.306902396D+05-3.028332772D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9014.108
-1.104748482D+09 3.561451690D+05-1.236258085D+01-2.812895475D-03 3.310897210D-07
-1.254960778D-11 1.696392420D-16                -3.157682531D+06 2.067297489D+02
BaO+              Gurvich,1996a pt1 p552 pt2 p421.
 3 g11/98 BA  1.00O   1.00E  -1.00    0.00    0.00 0  153.3258514     511704.686
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9469.786
 3.566410970D+05-3.779246710D+03 1.673544137D+01-1.306611610D-02 2.686157445D-06
 4.044077950D-09-2.016508813D-12                 7.983268490D+04-7.285118550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9469.786
-3.317679230D+05 1.594253495D+03 3.227247810D+00 5.722641500D-04-1.147415658D-07
 1.382873231D-11-6.384437030D-16                 5.025247610D+04 1.409092365D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9469.786
-3.283193020D+06 2.046049762D+03 4.048225140D+00 9.872145390D-05 7.763808620D-11
 2.536329860D-13-1.334411326D-18                 4.456858530D+04 8.528620900D+00
BaOH              Gurvich,1996a pt1 p557 pt2 p425.
 2 tpis96 BA  1.00O   1.00H   1.00    0.00    0.00 0  154.3343400    -224256.513
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11224.581
 3.776231510D+04-8.891390220D+02 9.531718000D+00-5.458825900D-03 4.941783010D-06
-1.809327537D-09 2.050048305D-13                -2.441852965D+04-2.489410158D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11224.581
 2.637336694D+06-8.365410400D+03 1.599803975D+01-5.098446050D-03 1.594657431D-06
-2.180478542D-10 1.084610688D-14                 2.393550647D+04-7.490705790D+01
BaOH+             Gurvich,1996a pt1 p558 pt2 p426.
 2 tpis96 BA  1.00O   1.00H   1.00E  -1.00    0.00 0  154.3337914     202019.313
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11302.980
 2.797632165D+04-7.680769400D+02 9.052978440D+00-4.368577900D-03 3.523497260D-06
-8.386360870D-10-6.475457470D-14                 2.623280802D+04-2.264561641D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11302.980
 8.766738430D+05-2.335819600D+03 7.973166060D+00 1.038679898D-04-6.319485780D-08
 1.028729445D-11-5.741808570D-16                 3.772517470D+04-1.930805001D+01
Ba(OH)2           Gurvich,1996a pt1 p561 pt2 p428.
 2 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 0  171.3416800    -606666.472
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17388.725
 5.702814900D+04-1.577384797D+03 1.659935325D+01-1.039598275D-02 9.664889600D-06
-3.673621440D-09 4.625784990D-13                -6.835158900D+04-5.851911700D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17388.725
 1.762908112D+06-4.676205420D+03 1.395135494D+01 2.051842928D-04-1.257265530D-07
 2.048917625D-11-1.144045777D-15                -4.545964410D+04-4.929457190D+01
BaS               Gurvich,1996a pt1 p585 pt2 p444.
 2 tpis96 BA  1.00S   1.00    0.00    0.00    0.00 0  169.3920000     38871.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9556.115
 1.377075147D+04-3.293500560D+02 5.811545840D+00-2.848973760D-03 3.576336020D-06
-2.325649347D-09 6.172805310D-13                 4.964432450D+03-3.497962615D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9556.115
 6.104262070D+06-2.227617479D+04 3.597513510D+01-2.157793740D-02 7.319872350D-06
-1.089038636D-09 5.884101950D-14                 1.404138006D+05-2.141776331D+02
Ba2               Gurvich,1996a pt1 p545 pt2 p417.
 2 tpis96 BA  2.00    0.00    0.00    0.00    0.00 0  274.6540000     355964.337
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11359.137
-1.294177083D+04-7.276330080D+02 1.464866569D+01-3.966331650D-02 5.898711060D-05
-4.235300560D-08 1.189594362D-11                 4.386712230D+04-4.145673670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11359.137
 2.160114547D+05 1.950676877D+02 2.253699771D+00 1.507750613D-04-4.742515000D-08
 7.048951960D-12-3.547440170D-16                 4.167762970D+04 2.375906459D+01
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Appendix D (*continued*)

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Be                Hf:Cox,1989. Kramida,1997. Gordon,1999.
 3 g11/97 BE  1.00    0.00    0.00    0.00    0.00 0    9.0121820     324000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-4.112901520D-04 5.364967360D-06 2.499999972D+00 7.569203690D-11-1.097852652D-13
 8.002110240D-17-2.303022777D-20                 3.822264590D+04 2.146172983D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-6.926285840D+05 2.466773005D+03-9.776613340D-01 2.458939515D-03-9.047950420D-07
 1.587880407D-10-9.415600603D-15                 2.300212917D+04 2.623234754D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.145833520D+08-2.254147519D+05 4.411437910D+01-3.022853591D-03 1.178346131D-07
-2.273387650D-12 1.196838345D-17                 1.866686325D+06-3.752337400D+02
Be+               Moore,1971. Moore,1970a. Gordon,1999.
 3 g 1/98 BE  1.00E  -1.00    0.00    0.00    0.00 0    9.0116334    1229701.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.471528569D+05 2.839228698D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-9.478135980D+04 2.768325398D+02 2.191388413D+00 1.648824289D-04-4.280166820D-08
 4.542350470D-12-6.270417825D-17                 1.453850986D+05 5.055503840D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.321269508D+08 1.525464518D+05-3.651092580D+01 4.812692090D-03-2.928878120D-07
 8.899649840D-12-1.055676610D-16                -1.052744318D+06 3.402173130D+02
Be++              Moore,1970a. Gordon,1999.
 3 g 3/97 BE  1.00E  -2.00    0.00    0.00    0.00 0    9.0110848    2993001.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.592279160D+05 2.145990203D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.592279160D+05 2.145990203D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.592279160D+05 2.145990203D+00
BeBr              Gurvich,1996a pt1 p374 pt2 p300.
 2 tpis96 BE  1.00BR  1.00    0.00    0.00    0.00 0   88.9161820     132446.308
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8971.108
 3.746288060D+04-4.722339070D+02 5.039409040D+00 5.798853220D-04-1.937634343D-06
 1.793372625D-09-5.672295580D-13                 1.723135679D+04-2.573912886D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8971.108
 8.217238140D+05-2.850509348D+03 8.017266020D+00-2.105663212D-03 6.849136340D-07
-9.989129320D-11 5.192456840D-15                 3.229372870D+04-2.326810811D+01
BeBr2             Gurvich,1996a pt1 p377 pt2 p302.
 2 tpis96 BE  1.00BR  2.00    0.00    0.00    0.00 0  168.8201820    -234062.499
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12837.501
-2.118698678D+04 2.090382611D+02 3.731171310D+00 1.115501549D-02-1.542821761D-05
 1.052354444D-08-2.850006057D-12                -3.090456277D+04 9.458917720D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12837.501
-1.041331811D+05-1.543443092D+02 7.614465410D+00-4.556700630D-05 1.003180548D-08
-1.146879501D-12 5.301795380D-17                -2.984527608D+04-1.149360980D+01
BeCL              Gurvich,1996a pt1 p369, pt2 p295.
 2 tpis96 BE  1.00CL  1.00    0.00    0.00    0.00 0   44.4651820      56693.107
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8861.107
 2.016138947D+04-1.413988978D+02 2.898223773D+00 6.069925510D-03-9.162038470D-06
 6.612620660D-09-1.859126853D-12                 6.626691440D+03 7.900181050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8861.107
 2.808845146D+05-1.103100122D+03 5.671189830D+00-5.443000450D-04 1.459036606D-07
-1.230971735D-11 9.900804760D-17                 1.224649804D+04-8.382371370D+00
BeCL2             Gurvich,1996a pt1 p373 pt2 p298.
 2 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 0   79.9181820     -361539.140
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12080.860
-2.229957657D+04 1.528781667D+02 3.714994710D+00 1.067776550D-02-1.397766942D-05
 9.066693560D-09-2.350292311D-12                -4.590428230D+04 6.682555572D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12080.860
-1.154087460D+05-2.484300053D+02 7.685672140D+00-7.444960370D-05 1.649479787D-08
-1.895997075D-12 8.804973950D-17                -4.468747280D+04-1.500337407D+01
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BeF               Gurvich,1996a pt1 p363, pt2 p291.
 2 tpis96 BE  1.00F   1.00     0.00     0.00     0.00 0   28.0105852    -170624.795
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8711.105
-4.664497230D+04 7.887178850D+02-1.463363201D+00 1.381790494D-02-1.591299964D-05
 9.352931520D-09-2.229211181D-12                 -2.522627476D+04 3.197634300D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8711.105
-1.857941543D+05 4.776082770D+01 4.269986020D+00 2.310668473D-04-6.657214920D-08
 1.152149888D-11-6.335586440D-16                 -2.257950960D+04-2.184787270D-01
BeF2              Gurvich,1996a pt1 p366 pt2 p293.
 2 tpis96 BE  1.00F   2.00     0.00     0.00     0.00 0   47.0089884    -796588.236
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10879.764
 7.490270240D+03-2.878053102D+02 5.434712820D+00 3.903233460D-03-2.214865601D-06
-1.965806119D-10 4.042362270D-13                 -9.591615640D+04-5.616616920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10879.764
-6.482018070D+04-7.684556060D+02 8.062860840D+00-2.227502549D-04 4.891598660D-08
-5.587886720D-12 2.583409761D-16                 -9.395495490D+04-2.125660266D+01
BeH               Gurvich,1996a pt1 p356, pt2 p286.
 2 tpis96 BE  1.00H   1.00     0.00     0.00     0.00 0   10.0201220     342252.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8648.104
-1.615149125D+03-5.935286080D+01 4.507269100D+00-5.264189610D-03 1.145319967D-05
-9.247883590D-09 2.700364753D-12                  4.030193040D+04-3.485117050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8648.104
-2.424081636D+06 6.597398460D+03-3.626316480D+00 4.579634350D-03-1.163329056D-06
 1.297785691D-10-5.291885810D-15                 -2.489846221D+03 5.216018690D+01
BeH+              Chase,1998 p391 9/66.
 3 g 1/01 BE  1.00H   1.00E  -1.00     0.00     0.00 0   10.0195734    1178218.951
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8643.951
-3.220611020D+04 2.520229596D+02 3.207719570D+00-2.191287290D-03 6.902534490D-06
-5.769522630D-09 1.656414969D-12                  1.392530660D+05 3.307044770D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8643.951
 4.622341590D+05-1.760169629D+03 5.379905550D+00 2.742462444D-05-1.167208170D-07
 3.557177910D-11-2.569695765D-15                  1.515859734D+05-1.369222641D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8643.951
 2.282300776D+08-1.214880850D+05 2.642762928D+01-1.410369386D-03 3.776812140D-08
 6.975949060D-14-1.287263021D-17                  1.127119075D+06-2.060147218D+02
BeH2              Martin,1992. Martin,1997.
 2 g 4/01 BE  1.00H   2.00     0.00     0.00     0.00 0   11.0280620     161098.903
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9219.103
 9.065314900D+04-1.320657220D+03 9.901308060D+00-1.255772231D-02 2.205704068D-05
-1.633609388D-08 4.505103240D-12                  2.464561869D+04-3.635826750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9219.103
 6.074262010D+05-3.407534250D+03 9.792370360D+00-8.254614820D-04 1.915656246D-07
-1.962774813D-11 8.929908660D-16                  3.793105200D+04-4.254653580D+01
BeI               Gurvich,1996a pt1 p378, pt2 p303.
 2 tpis96 BE  1.00I   1.00     0.00     0.00     0.00 0  135.9166520     207454.309
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9089.109
 3.530054810D+04-5.190950260D+02 5.714505240D+00-1.409073640D-03 7.664772120D-07
-2.601945105D-11-8.230960640D-14                  2.637903657D+04-5.140997840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9089.109
-5.328206620D+05 1.139497861D+03 3.629171660D+00 1.704033769D-04 1.067048688D-07
-3.589457880D-11 2.722769560D-15                  1.585474307D+04 9.370951270D+00
BeI2              Gurvich,1996a pt1 p380 pt2 p305.
 2 tpis96 BE  1.00I   2.00     0.00     0.00     0.00 0  262.8211220     -64759.451
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13440.549
 3.592726180D+02-4.866059010D+01 5.241571180D+00 7.830305060D-03-1.169525374D-05
 8.389583910D-09-2.356636003D-12                 -9.333220920D+03 2.896318281D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13440.549
-9.392372840D+04-8.959214380D+01 7.565554790D+00-2.577727326D-05 5.614265330D-09
-6.359663850D-13 2.917080336D-17                 -9.814768620D+03-9.032042810D+00
BeN               Chase,1998 p403.
 2 j 6/63 BE  1.00N   1.00     0.00     0.00     0.00 0   23.0188820     427000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8725.221
-4.247783630D+04 7.590188900D+02-1.561469235D+00 1.496945721D-02-1.835608880D-05
 1.146861461D-08-2.897470581D-12                  4.683003320D+04 3.256973759D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8725.221
-5.909696160D+04-3.078649431D+02 4.727959150D+00-3.928158830D-05 2.006201069D-08
-2.300018068D-12 1.066101831D-16                  5.156095710D+04-3.031380625D+00
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Appendix D (*continued*)

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BeO                Gurvich,1996a pt1 p351, pt2 p280.
 3 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 0   25.0115820     128940.304
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8688.104
-4.869458320D+04 7.213473620D+02-3.784157320D-01 8.792203850D-03-7.070151260D-06
 2.250175620D-09-2.799117872D-14                 1.101466639D+04 2.574081184D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8688.104
-3.503472450D+07 1.055859473D+05-1.165011722D+02 6.477369480D-02-1.649656058D-05
 2.005558400D-09-9.426891790D-14                -6.570018000D+05 8.640898030D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8688.104
-7.440106320D+07 4.309665300D+04-1.019586064D-01 2.617209088D-04-2.461810861D-08
 1.124733698D-12-1.832802285D-17                -3.402379380D+05 4.487040230D+01
BeOH               Gurvich,1996a pt1 p358 pt2 p288.
 2 tpis96 BE  1.00O   1.00H   1.00    0.00    0.00 0   26.0195220     -99717.721
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10798.450
-3.853024520D+04 4.498059290D+02 1.532096459D+00 1.299912603D-02-1.708979996D-05
 1.169968182D-08-3.163183710D-12                -1.559046567D+04 1.545542930D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10798.450
 8.550330310D+05-2.646537838D+03 8.204784630D+00 1.110814513D-05-4.265364000D-08
 7.926511920D-12-4.645419520D-16                 3.121216271D+03-2.571641308D+01
BeOH+              Chase,1998 p393.
 3 j12/75 BE  1.00O   1.00H   1.00E  -1.00    0.00 0   26.0189734     759983.920
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9550.904
 7.106119160D+04-8.068981600D+02 5.603107810D+00 4.932070860D-03-7.722847160D-06
 5.910889810D-09-1.695201901D-12                 9.440782420D+04-1.088099852D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9550.904
 8.134874390D+05-2.814653683D+03 8.381145010D+00-6.942073280D-05-2.369535806D-08
 5.678106380D-12-3.583253560D-16                 1.073129932D+05-2.901093335D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9550.904
-6.279111750D+06 2.090044240D+03 7.025559910D+00 5.492111300D-05-3.446137200D-09
 1.115947764D-13-1.461494242D-18                 6.914837000D+04-1.732443156D+01
Be(OH)2            Gurvich,1996a pt1 p360 pt2 p290.
 2 tpis96 BE  1.00O   2.00H   2.00    0.00    0.00 0   43.0268620    -638864.416
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15225.858
 7.863089830D+03-7.397142250D+02 1.043303334D+01 4.514249530D-03-6.950601530D-06
 5.777030040D-09-1.727199382D-12                -7.585676960D+04-3.301466610D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15225.858
 1.722889403D+06-5.242477190D+03 1.486877785D+01 3.931498360D-05-8.920276310D-08
 1.630912925D-11-9.505371140D-16                -4.642823840D+04-6.476804020D+01
BeS                Gurvich,1996a pt1 p381 pt2 p307.
 2 tpis96 BE  1.00S   1.00    0.00    0.00    0.00 0   41.0771820     247095.306
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8780.106
-7.390579080D+03 2.828134792D+02 6.552019400D-01 1.076012495D-02-1.398380157D-05
 8.818418890D-09-2.110588578D-12                 2.751593294D+04 1.980493561D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8780.106
-1.655708361D+07 5.431466120D+04-6.351859250D+01 3.964091990D-02-1.078978696D-05
 1.394030343D-09-6.936955040D-14                -3.121559628D+05 4.803454935D+02
Be2                Gurvich,1996a pt1 p346 pt2 p277.
 2 tpis96 BE  2.00    0.00    0.00    0.00    0.00 0   18.0243640     637543.318
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9838.118
-1.580873810D+05 2.035567774D+03-3.691580630D+00 1.028818435D-02-9.603854510D-06
 4.707519420D-09-9.374688790D-13                 6.526968370D+04 4.879324990D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9838.118
 1.010034484D+05 1.414207488D+02 2.292070182D+00 1.543331824D-04-5.801043000D-08
 1.003129697D-11-5.682818340D-16                 7.550139730D+04 1.238758616D+01
Be2CL4             Gurvich,1996a pt1 p374 pt2 p299.
 2 tpis96 BE  2.00CL  4.00    0.00    0.00    0.00 0  159.8363640    -819604.973
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22641.384
 1.216152589D+05-2.000824823D+03 1.723384275D+01 5.810448280D-03-1.362970089D-05
 1.156602362D-08-3.552255800D-12                -9.206475470D+04-6.137959774D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22641.384
-3.354920080D+05-2.316199283D+02 1.617047912D+01-6.734405950D-05 1.472073032D-08
-1.672352806D-12 7.688773970D-17                -1.031075197D+05-5.047009374D+01
Be2F4              Gurvich,1996a pt1 p368 pt2 p294.
 2 tpis96 BE  2.00F   4.00    0.00    0.00    0.00 0   94.0179768   -1731699.842
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19834.508
-6.327701870D+03-6.902533720D+01 5.470937230D+00 3.097341347D-02-4.094310060D-05
 2.668113685D-08-6.942909560D-12                -2.105979269D+05-2.073546195D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19834.508
-3.681834950D+05-9.439191480D+02 1.670099855D+01-2.797974015D-04 6.178061720D-08
-7.083080190D-12 3.282791040D-16                -2.089045725D+05-6.092665760D+01
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Appendix D (*continued*)

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Be2O              Gurvich,1996a pt1 p353 pt2 p282.
 2 tpis96 BE  2.00O   1.00     0.00     0.00     0.00 0   34.0237640      -37033.803
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11190.386
-4.263673570D+02-1.159556261D+02 4.082677770D+00 1.015885064D-02-1.326015538D-05
 8.488955360D-09-2.168039077D-12                 -5.362258120D+03 1.253737886D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11190.386
-1.412646378D+05-3.498644590D+02 7.760932680D+00-1.044953518D-04 2.313342334D-08
-2.657722263D-12 1.233820439D-16                 -5.172385490D+03-1.854887619D+01
Be2OF2            Chase,1998 p417.
 2 j 6/66 BE  2.00O   1.00F    2.00     0.00     0.00 0   72.0205704    -1204574.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16584.874
-2.783491921D+04 1.782881461D+02 4.094251360D+00 2.270142496D-02-2.672688189D-05
 1.572575618D-08-3.736070580D-12                 -1.480081903D+05 7.353494770D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16584.874
-2.281826506D+05-1.130355396D+03 1.383400563D+01-3.316080640D-04 7.304921010D-08
-8.362704380D-12 3.872184980D-16                 -1.431390587D+05-4.739150230D+01
Be2O2             Gurvich,1996a pt1 p354 pt2 p283.
 2 tpis96 BE  2.00O   2.00     0.00     0.00     0.00 0   50.0231640     -411635.309
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10928.932
-3.031719530D+04 1.163353177D+03-8.733155950D+00 5.372002930D-02-7.279439190D-05
 4.894928250D-08-1.312147056D-11                 -5.546936880D+04 6.953282640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10928.932
-3.960576640D+05-9.074948830D+02 1.067160422D+01-2.670905218D-04 5.877629990D-08
-6.718664090D-12 3.105949075D-16                 -4.861114330D+04-3.616546890D+01
Be3O3             Gurvich,1996a pt1 p355 pt2 p284.
 2 tpis96 BE  3.00O   3.00     0.00     0.00     0.00 0   75.0347460    -1023720.628
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15125.733
-2.738072346D+04 8.743832600D+02-6.599606120D+00 6.533021140D-02-8.762305740D-05
 5.817244790D-08-1.540600500D-11                 -1.284679012D+05 5.837203120D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15125.733
-5.890809360D+05-1.392823588D+03 1.703450699D+01-4.127330740D-04 9.107529150D-08
-1.043465231D-11 4.833053770D-16                 -1.219045534D+05-7.000614510D+01
Be4O4             Gurvich,1996a pt1 p356 pt2 p285.
 2 tpis96 BE  4.00O   4.00     0.00     0.00     0.00 0  100.0463280    -1649294.582
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15833.899
-6.893255640D+04 1.687565069D+03-1.479616594D+01 1.007319774D-01-1.291057622D-04
 8.243136760D-08-2.111283987D-11                 -2.072877151D+05 1.002507262D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15833.899
-8.841338460D+05-2.726394165D+03 2.402941774D+01-8.114675460D-04 1.794255972D-07
-2.059359498D-11 9.552905330D-16                 -1.923710587D+05-1.136620750D+02
Br                Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 3/97 BR  1.00    0.00     0.00     0.00     0.00 0   79.9040000     111870.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-3.700293910D+03 6.145215420D+01 2.092120721D+00 1.376818870D-03-2.445566658D-06
 2.050975161D-09-5.144249091D-13                  1.242508647D+04 8.996166200D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-4.789717400D+06 1.692051999D+04-2.024085357D+01 1.395620355D-02-3.656230560D-06
 4.489781000D-10-2.122507526D-14                 -9.207054960D+04 1.661695929D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-1.240248003D+08 7.034034730D+04-1.023087313D+01 1.373755814D-03-7.476473480D-08
 2.160883187D-12-2.659054603D-17                 -5.563101070D+05 1.226657143D+02
Br+               Moore,1971. Moore,1970a. Gordon,1999.
 3 g10/97 BR  1.00E  -1.00     0.00     0.00     0.00 0   79.9034514    1257927.034
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.434
 3.981187420D+04-4.751581470D+02 4.734578980D+00-5.169324790D-03 5.905857520D-06
-2.885129283D-09 5.054894290D-13                  1.529052046D+05-5.769283220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.434
 1.741149829D+06-5.455465670D+03 8.470663350D+00-2.683465574D-03 6.590454560D-07
-7.953770300D-11 3.735898818D-15                  1.851781643D+05-3.637909030D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.434
-6.174903280D+07 3.641704160D+04-5.739744680D+00 1.067497350D-03-7.127689890D-08
 2.155618820D-12-1.769476126D-17                 -1.399767498D+05 7.931577700D+01
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Br-                Hotop,1985. Gordon,1999.
 3 g10/97 BR  1.00E   1.00     0.00     0.00     0.00 0   79.9045486     -219000.472
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.708492743D+04 5.419556170D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.708492743D+04 5.419556170D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.708492743D+04 5.419556170D+00
BrCL               Gurvich,1989 pt1 p213 pt2 p112.
 2 tpis89 BR  1.00CL  1.00     0.00     0.00     0.00 0  115.3570000      14789.113
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9407.113
 1.653291583D+04-3.578769280D+02 5.700622160D+00-2.201257188D-03 2.415146969D-06
-1.371032976D-09 3.227803420D-13                 2.252619279D+03-4.155659669D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9407.113
-1.284863067D+05-1.138379626D+03 7.964040800D+00-3.438056670D-03 1.524999514D-06
-2.761469114D-10 1.694450407D-14                 5.938264260D+03-1.925044389D+01
BrF                Gurvich,1989 pt1 p208 pt2 p109.
 2 tpis89 BR  1.00F   1.00     0.00     0.00     0.00 0   98.9024032     -58851.445
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9021.108
 3.836143190D+04-5.184611970D+02 5.458327050D+00-5.656843100D-04-4.121311970D-07
 7.859913480D-10-3.036161520D-13                -5.595539910D+03-4.901129500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9021.108
 3.771388470D+06-1.267493430D+04 2.080555930D+01-1.026359360D-02 3.308203590D-06
-4.903192250D-10 2.648275080D-14                 7.062609720D+04-1.130253600D+02
BrF3               Gurvich,1989 pt1 p211 pt2 p110.
 2 tpis89 BR  1.00F   3.00     0.00     0.00     0.00 0  136.8992096     -255600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14711.620
 1.116455127D+05-1.959424330D+03 1.526220126D+01-7.999362300D-03 6.982030260D-06
-3.242757960D-09 6.164751460D-13                -2.345341551D+04-5.522633600D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14711.620
-1.886532240D+05-8.245232970D+01 1.006180694D+01-2.477319092D-05 5.478576860D-09
-6.282655260D-13 2.910628214D-17                -3.386800370D+04-2.298937369D+01
BrF5               Gurvich,1989 pt1 p212 pt2 p111.
 2 tpis89 BR  1.00F   5.00     0.00     0.00     0.00 0  174.8960160     -428800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19174.543
 2.211366805D+05-4.024809220D+03 2.734900212D+01-1.832254979D-02 1.721754649D-05
-8.753508630D-09 1.860196959D-12                -3.537447670D+04-1.244296466D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19174.543
-3.757647640D+05-1.575896472D+02 1.611869838D+01-4.776497800D-05 1.059755365D-08
-1.218527723D-12 5.657535450D-17                -5.667266800D+04-5.540839310D+01
BrO                Chase,1996a.
 2 j 3/96 BR  1.00O   1.00     0.00     0.00     0.00 0   95.9034000     125800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9061.000
 1.455431116D+04 1.225152439D+02-3.058728672D-01 2.117309202D-02-3.494261190D-05
 2.622639719D-08-7.508059540D-12                 1.389149932D+04 2.527867438D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9061.000
-2.392612795D+06 6.932793130D+03-2.513183892D+00 3.446544560D-03-7.569536840D-07
 6.514291340D-11-1.715768736D-15                -3.084499064D+04 5.361048360D+01
OBrO               Chase,1996a.
 2 j 3/96 BR  1.00O   2.00     0.00     0.00     0.00 0  111.9028000     151954.526
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11394.630
 3.470213230D+04-3.401341820D+02 3.932251620D+00 1.215938586D-02-1.901501702D-05
 1.398631495D-08-3.992899760D-12                 1.875955788D+04 6.361235180D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11394.630
-1.624504660D+05-1.453689372D+02 7.105822130D+00-4.141362070D-05 8.981833260D-09
-1.013712869D-12 4.635133140D-17                 1.650075386D+04-9.111817920D+00
BrOO               Chase,1996a.
 2 j 3/96 BR  1.00O   2.00     0.00     0.00     0.00 0  111.9028000     108000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12850.660
-4.417619900D+04 4.959637160D+02 3.239884950D+00 5.941502110D-03-3.402696770D-06
-3.444778160D-11 4.811957950D-13                 8.815221980D+03 1.607446878D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12850.660
 6.172483480D+03-6.585049660D+02 7.483955330D+00-1.920530746D-04 4.226946170D-08
-4.837392610D-12 2.239741320D-16                 1.460353470D+04-9.850380240D+00
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BrO3                Chase,1996a.
 2 j 3/96 BR  1.00O   3.00     0.00     0.00     0.00 0  127.9022000      220820.685
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13100.841
 1.063901881D+05-1.501928813D+03 9.703657430D+00 8.133000760D-03-1.531857845D-05
 1.199117619D-08-3.512747870D-12                 3.233135990D+04-2.735125430D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13100.841
-2.822851113D+05-2.358973461D+02 1.017525279D+01-6.978451050D-05 1.535701661D-08
-1.754454950D-12 8.104100150D-17                 2.401140140D+04-2.588197197D+01
Br2                 Gurvich,1989 pt1 p200 pt2 p104.
 2 tpis89 BR  2.00    0.00     0.00     0.00     0.00 0  159.8080000      30910.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9725.117
 7.497047540D+03-2.350884557D+02 5.491934320D+00-2.227573303D-03 2.932401703D-06
-1.954889514D-09 5.312307890D-13                 3.521475050D+03-1.964151570D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9725.117
-4.311698570D+06 1.111268634D+04-5.555775610D+00 3.630516590D-03-2.754164226D-07
-6.217506760D-11 7.375341620D-15                -7.036584160D+04 7.878478020D+01
BrBrO               Chase,1996a.
 2 j 3/96 BR  2.00O   1.00     0.00     0.00     0.00 0  175.8074000      168000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13137.498
 1.617498037D+04-2.464406776D+02 5.912858450D+00 4.980354280D-03-8.099958250D-06
 6.072776260D-09-1.753715313D-12                 1.974012093D+04 2.009704963D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13137.498
-8.537101750D+04-6.487046070D+01 7.047159350D+00-1.843088186D-05 3.992267860D-09
-4.500687950D-13 2.055867395D-17                 1.821566655D+04-3.162186125D+00
BrOBr               Chase,1996a.
 2 j 3/96 BR  2.00O   1.00     0.00     0.00     0.00 0  175.8074000      107639.006
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12399.058
 6.405068910D+04-1.062722566D+03 9.907866290D+00-4.470492470D-03 3.913701070D-06
-1.805444867D-09 3.366132550D-13                 1.642921537D+04-2.350319399D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12399.058
-9.686660250D+04-3.957395270D+01 7.029434380D+00-1.171881908D-05 2.576958549D-09
-2.941186078D-13 1.357198784D-17                 1.076942321D+04-5.697779380D+00
C                   Hf:Douglas,1955. Moore,1970b. Gordon,1999.
 3 g 7/97 C   1.00     0.00     0.00     0.00     0.00 0   12.0107000      716680.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6535.895
 6.495031470D+02-9.649010860D-01 2.504675479D+00-1.281448025D-05 1.980133654D-08
-1.606144025D-11 5.314483411D-15                 8.545763110D+04 4.747924288D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6535.895
-1.289136472D+05 1.719528572D+02 2.646044387D+00-3.353068950D-04 1.742092740D-07
-2.902817829D-11 1.642182385D-15                 8.410597850D+04 4.130047418D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6535.895
 4.432528010D+08-2.886018412D+05 7.737108320D+01-9.715281890D-03 6.649595330D-07
-2.230078776D-11 2.899388702D-16                 2.355273444D+06-6.405123160D+02
C+                  Moore,1970b. Gordon,1999.
 3 g 6/98 C   1.00E  -1.00     0.00     0.00     0.00 0   12.0101514     1809444.482
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6649.282
 2.258535929D+03-1.574575687D+00 2.503637730D+00-5.202878370D-06 4.516908390D-09
-2.181431053D-12 4.495047033D-16                 2.168951913D+05 4.345699505D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6649.282
 1.255112551D+04-3.411874670D+01 2.543383218D+00-2.805120849D-05 9.751641970D-09
-1.736855394D-12 1.246191931D-16                 2.171001786D+05 4.063913515D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6649.282
 5.618135320D+05-6.047058900D+03 5.884541470D+00-7.211894530D-04 6.823484110D-08
-2.599878590D-12 3.633868358D-17                 2.581370458D+05-2.280019759D+01
C-                  Hotop,1985. Gordon,1999.
 3 g 3/98 C   1.00E   1.00     0.00     0.00     0.00 0   12.0112486      588314.236
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6218.836
 4.671291530D+00-1.986169369D-03 2.500008638D+00-1.976750928D-08 2.478947477D-11
-1.610664044D-14 4.236506810D-18                 7.001218550D+04 4.879570141D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6218.836
 4.253175720D+00 5.778186480D-04 2.499999424D+00 2.836136231D-10-7.327253420D-14
 9.478507810D-18-4.830487320D-22                 7.001217170D+04 4.879624211D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6218.836
 1.223289007D+01-5.196185830D-03 2.500001344D+00-1.743497251D-10 1.206609009D-14
-4.252419790D-19 5.992333270D-24                 7.001221630D+04 4.879608421D+00
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Appendix D (*continued*)

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CBr                Gurvich,1991 pt1 p157 pt2 p137.
 2 tpis91 C    1.00BR  1.00     0.00     0.00     0.00 0    91.9147000      490431.816
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9615.116
 4.324446880D+03-1.596366559D+02 4.857856590D+00-4.389439160D-04 4.408863630D-07
-2.281330618D-10 5.445618220D-14                 5.847677250D+04 1.351169646D-01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9615.116
 1.021862102D+06-3.243484360D+03 8.388226560D+00-2.242155508D-03 6.988355370D-07
-9.719134370D-11 4.716976240D-15                 7.805924060D+04-2.518386915D+01
CBr2               Gurvich,1991 pt1 p159 pt2 p138.
 2 tpis91 C    1.00BR  2.00     0.00     0.00     0.00 0   171.8187000      336623.319
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12196.819
 7.248197840D+04-1.128261230D+03 9.822303380D+00-3.872748100D-03 2.904819596D-06
-1.061380159D-09 1.297474642D-13                 4.437771600D+04-2.361121795D+01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12196.819
-7.441431410D+05 4.215427830D+02 8.796797740D+00-2.726562507D-03 1.336438546D-06
-2.304854483D-10 1.337493953D-14                 3.364618140D+04-1.599565135D+01
CBr3               Gurvich,1991 pt1 p160 pt2 p139.
 2 tpis91 C    1.00BR  3.00     0.00     0.00     0.00 0   251.7227000      235000.000
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15582.455
 8.563516260D+04-1.275764123D+03 1.117190031D+01 2.341705749D-03-6.540671410D-06
 5.736717140D-09-1.777823046D-12                 3.243215890D+04-2.766468801D+01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15582.455
-1.926498949D+05-1.324072178D+02 1.009808665D+01-3.895040820D-05 8.550445010D-09
-9.747493680D-13 4.494245590D-17                 2.541576129D+04-1.866868947D+01
CBr4               Kudchadker,1975.
 2 g 8/99 C    1.00BR  4.00     0.00     0.00     0.00 0   331.6267000       79500.000
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20373.314
 1.023083739D+05-1.735600709D+03 1.651317914D+01-3.147664747D-03 2.924135486D-07
 1.360605681D-09-6.431758650D-13                 1.500502543D+04-5.536476760D+01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20373.314
-2.059785072D+05-1.048517002D+02 1.307772550D+01-3.086857556D-05 6.775309810D-09
-7.721837540D-13 3.559218240D-17                 5.615893940D+03-3.283787630D+01
CCL                Hf:Kumaran,1997. Gurvich,1991 pt1 p106 pt2 p81.
 2 g 8/99 C    1.00CL  1.00     0.00     0.00     0.00 0    47.4637000      432611.058
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9395.113
 1.707070049D+04-1.463803497D+01 2.334108251D+00 7.202099130D-03-1.034120045D-05
 7.228106700D-09-1.985123755D-12                 5.123350300D+04 1.200820386D+01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9395.113
 5.900507630D+05-2.075311460D+03 6.880017230D+00-1.294796228D-03 3.883137980D-07
-5.006981630D-11 2.218229619D-15                 6.358922050D+04-1.610664472D+01
CCLBr3             Gurvich,1991 pt1 p171 pt2 p152.
 2 tpis91 C    1.00CL  1.00BR  3.00     0.00     0.00 0   287.1757000       65000.000
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19568.242
 1.021596752D+05-1.746281176D+03 1.598215634D+01-1.350975234D-03-2.330039129D-06
 3.201856270D-09-1.150412393D-12                 1.341967771D+04-5.285079043D+01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19568.242
-2.282709343D+05-1.277037936D+02 1.309470658D+01-3.763326710D-05 8.264715600D-09
-9.424237560D-13 4.345940760D-17                 3.930463310D+03-3.315414033D+01
CCL2               Hf:Kumaran,1997. Jacox,1994. Shin,1990.
 2 g 8/99 C    1.00CL  2.00     0.00     0.00     0.00 0    82.9167000      222940.147
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11422.758
 7.509623150D+04-1.034728559D+03 8.061704540D+00 1.487134213D-03-4.564817110D-06
 3.954885810D-09-1.166197091D-12                 3.052409293D+04-1.739691692D+01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11422.758
-6.437455170D+06 1.958413353D+04-1.604038625D+01 1.238833906D-02-3.013367274D-06
 3.473468920D-10-1.553272793D-14                -9.961242160D+04 1.556949315D+02
CCL2Br2            Gurvich,1991 pt1 p170 pt2 p151.
 2 tpis91 C    1.00CL  2.00BR  2.00     0.00     0.00 0   242.7247000       10000.000
    200.000    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18691.912
 1.018495619D+05-1.740854039D+03 1.521338304D+01 1.128256510D-03-5.875405490D-06
 5.659886970D-09-1.821576512D-12                 6.918572190D+03-5.015385819D+01
   1000.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18691.912
-2.553347012D+05-1.598005477D+02 1.311860930D+01-4.717443870D-05 1.036912808D-08
-1.183321687D-12 5.460612690D-17                -2.588636980D+03-3.461705319D+01
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CCL3              Hf:Hudgens,1991. TRC(12/93) tuv7270.
 2 n12/93 C   1.00CL  3.00     0.00     0.00     0.00 0  118.3697000       71128.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14400.000
 3.414471650D+04-5.547969730D+02 6.845544390D+00 1.242006495D-02-2.036896881D-05
 1.554979993D-08-4.568940110D-12                 9.388568820D+03-7.143598465D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14400.000
-5.427572540D+05 6.809020620D+02 9.047723620D+00 1.324277766D-04 6.301263040D-08
-2.656639200D-11 2.105668053D-15                 3.866216150D+02-1.528745849D+01
CCL3Br            Gurvich,1991 pt1 p169 pt2 p150.
 2 tpis91 C   1.00CL  3.00BR  1.00     0.00     0.00 0  198.2737000      -43000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17984.549
 1.049668463D+05-1.793828482D+03 1.489250892D+01 2.397128310D-03-7.789615470D-06
 7.016617110D-09-2.196069746D-12                 9.101349310D+02-5.058348139D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17984.549
-2.772324186D+05-1.840310333D+02 1.313673812D+01-5.443910010D-05 1.197658923D-08
-1.367818632D-12 6.316164790D-17                -8.895857690D+03-3.669528209D+01
CCL4              Gurvich,1991 pt1 p111 pt2 p84.
 2 tpis91 C   1.00CL  4.00     0.00     0.00     0.00 0  153.8227000      -95600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17158.512
 1.093385626D+05-1.861731846D+03 1.449632467D+01 3.949485160D-03-1.010805379D-05
 8.645514170D-09-2.642368852D-12                -4.948006230D+03-5.180284750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17158.512
-3.043078255D+05-2.168170491D+02 1.316132386D+01-6.431124890D-05 1.416482497D-08
-1.619343320D-12 7.483974350D-17                -1.512320070D+04-3.996844300D+01
CF                Hf:TRC(6/88) w6950. Gurvich,1991 pt1 p74 pt2 p55.
 2 tpis91 C   1.00F   1.00     0.00     0.00     0.00 0   31.0091032      242300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9065.109
-4.582786680D+04 7.972635890D+02-1.364936319D+00 1.312359375D-02-1.457012892D-05
 8.253276680D-09-1.896351845D-12                 2.438259620D+04 3.248065280D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9065.109
-1.329807100D+05-1.214340891D+02 4.452413620D+00 1.293786948D-04-3.670550590D-08
 6.590212390D-12-3.731261610D-16                 2.815934108D+04-6.640468730D-01
CF+               Chase,1998 p579 12/70.
 2 g12/99 C   1.00F   1.00E  -1.00     0.00     0.00 0   31.0085546     1145564.099
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8697.499
-5.975213200D+04 9.276863650D+02-1.866581982D+00 1.384340912D-02-1.513428860D-05
 8.518556340D-09-1.959577655D-12                 1.323519410D+05 3.412013190D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8697.499
-8.053762780D+04-3.390275090D+02 4.708373500D+00-3.963148310D-05 2.497996218D-08
-5.236790430D-12 5.313949130D-16                 1.381337068D+05-3.920514730D+00
CFBr3             Gurvich,1991 pt1 p166 pt2 p146.
 2 tpis91 C   1.00F   1.00BR  3.00     0.00     0.00 0  270.7211032     -120000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18243.104
 5.149244280D+04-9.364796640D+02 1.044260886D+01 1.205370047D-02-1.876290291D-05
 1.344488618D-08-3.730545760D-12                -1.243246293D+04-2.363948551D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18243.104
-2.729158956D+05-3.328164650D+02 1.324822519D+01-9.927077540D-05 2.193640054D-08
-2.515424945D-12 1.165680878D-16                -1.730185479D+04-3.626818430D+01
CFCL              Hf:Gurvich,1991 pt1 p135 pt2 p107. Jacox,1994.
 2 g 9/99 C   1.00F   1.00CL  1.00     0.00     0.00 0   66.4621032       25845.774
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10902.382
 1.541997945D+04-8.274039810D+01 2.501701822D+00 1.390738086D-02-1.895734700D-05
 1.261934581D-08-3.333453820D-12                 2.411755114D+03 1.331517094D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10902.382
-2.681630077D+05-2.328091539D+00 6.834633830D+00 1.565270633D-04-5.967755160D-08
 9.820924460D-12-5.058897210D-16                 3.017669604D+02-9.005085129D+00
CFCLBr2           Gurvich,1991 pt1 p175 pt2 p158.
 2 tpis91 C   1.00F   1.00CL  1.00BR  2.00     0.00 0  226.2701032     -175000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17498.023
 5.898799740D+04-1.050714861D+03 1.039349401D+01 1.273690622D-02-1.999097478D-05
 1.438204230D-08-4.000130350D-12                -1.837799602D+04-2.417479131D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17498.023
-2.960811596D+05-3.531276200D+02 1.326346169D+01-1.053860298D-04 2.329085080D-08
-2.670979639D-12 1.237844667D-16                -2.387594306D+04-3.684977271D+01
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CFCL2            Gurvich,1991 pt1 p138 pt2 p110.
 2 tpis91 C   1.00F   1.00CL  2.00    0.00    0.00 0  101.9151032    -105000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13216.954
 2.611398792D+04-3.353565900D+02 4.094673080D+00 1.960244711D-02-2.762775193D-05
 1.880124302D-08-5.047410300D-12                 -1.251298871D+04 6.870882561D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13216.954
-2.653118323D+05-4.469724170D+02 1.033334881D+01-1.333673368D-04 2.948755634D-08
-3.383306200D-12 1.568746348D-16                 -1.393160489D+04-2.556817972D+01
CFCL2Br          Gurvich,1991 pt1 p175 pt2 p157.
 2 tpis91 C   1.00F   1.00CL  2.00BR  1.00    0.00 0  181.8191032    -235000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16730.573
 6.529959220D+04-1.135235485D+03 1.009526872D+01 1.401380147D-02-2.191705096D-05
 1.573404132D-08-4.369340340D-12                 -2.504488145D+04-2.451093103D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16730.573
-3.215455050D+05-3.884129620D+02 1.328990796D+01-1.160048581D-04 2.564498787D-08
-2.941639768D-12 1.363542881D-16                 -3.097421144D+04-3.871356695D+01
CFCL3            Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p140 pt2 p112.
 2 g 7/99 C   1.00F   1.00CL  3.00    0.00    0.00 0  137.3681032    -283700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16063.584
 7.400174000D+04-1.252282466D+03 1.001327229D+01 1.475107601D-02-2.315635251D-05
 1.664207025D-08-4.622929960D-12                 -3.020508601D+04-2.708387087D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16063.584
-3.450464780D+05-4.177821450D+02 1.331196736D+01-1.248759531D-04 2.761391353D-08
-3.168207640D-12 1.468834601D-16                 -3.674067190D+04-4.156886057D+01
CF2              Hf:TRC(6/88) w6950. Jacox,1998.
 2 g 9/99 C   1.00F   2.00    0.00    0.00    0.00 0   50.0075064    -186600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10350.912
-3.797026270D+04 8.731800030D+02-3.460191570D+00 2.746253741D-02-3.474621900D-05
 2.204470693D-08-5.621750850D-12                 -2.746797157D+04 4.456778070D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10350.912
-1.086428547D+05-5.854989140D+02 7.018648950D+00 3.929186150D-04-2.603822675D-07
 6.142196390D-11-4.172833260D-15                 -2.152945157D+04-1.356143285D+01
CF2+             Chase,1998 p583 12/70. Jacox,1994.
 2 g 9/99 C   1.00F   2.00E  -1.00    0.00    0.00 0   50.0069578     949341.299
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10341.999
-2.892373827D+04 6.049354610D+02-9.721866660D-01 1.808478341D-02-1.980065782D-05
 1.101640055D-08-2.500457119D-12                 1.102755670D+05 3.247591470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10341.999
-6.488966070D+04-1.064283593D+03 7.785702100D+00-3.158347626D-04 7.130804080D-08
-8.533183590D-12 4.251638820D-16                 1.178446465D+05-1.819424707D+01
CF2Br2           Gurvich,1991 pt1 p166 pt2 p145.
 2 tpis91 C   1.00F   2.00BR  2.00    0.00    0.00 0  209.8155064    -380000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16279.997
 1.261404028D+04-2.815725114D+02 5.098032130D+00 2.502548939D-02-3.438853190D-05
 2.297615553D-08-6.080161430D-12                 -4.642763750D+04 3.094167118D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16279.997
-3.327669300D+05-6.184352490D+02 1.346170049D+01-1.849172548D-04 4.092591340D-08
-4.699810430D-12 2.180811799D-16                 -4.715186610D+04-4.105369240D+01
CF2CL            Gurvich,1991 pt1 p136 pt2 p108.
 2 tpis91 C   1.00F   2.00CL  1.00    0.00    0.00 0   85.4605064    -275000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12432.273
 8.914558350D+03-1.768816959D+01 1.607015025D+00 2.473626554D-02-3.270738940D-05
 2.126351830D-08-5.509831110D-12                 -3.427306250D+04 1.929680690D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12432.273
-2.802346654D+05-6.860314850D+02 1.051143635D+01-2.046954963D-04 4.528897180D-08
-5.200229030D-12 2.412971450D-16                 -3.308179480D+04-2.874899785D+01
CF2CLBr          Gurvich,1991 pt1 p173 pt2 p156.
 2 tpis91 C   1.00F   2.00CL  1.00BR  1.00    0.00 0  165.3645064    -435000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15528.243
 2.696699365D+04-4.678832270D+02 5.244809420D+00 2.530121349D-02-3.508443520D-05
 2.354353958D-08-6.246161130D-12                 -5.198382730D+04 8.532887803D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15528.243
-3.592828840D+05-6.539283590D+02 1.348831524D+01-1.956099469D-04 4.329775970D-08
-4.972644370D-12 2.307575050D-16                 -5.365141170D+04-4.224913908D+01
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Appendix D (*continued*)

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CF2CL2              Hf:TRC(6/89) w7350.Gurvich,1991 pt1 p139 pt2 p111.
 2 g 7/99 C   1.00F   2.00CL  2.00     0.00     0.00 0  120.9135064     -490800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14881.094
 3.841258750D+04-6.139499820D+02 5.269667190D+00 2.574105783D-02-3.587376480D-05
 2.411600130D-08-6.402236900D-12                 -5.784541330D+04-1.957454856D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14881.094
-3.827448550D+05-6.933774800D+02 1.351791274D+01-2.075114435D-04 4.594021610D-08
-5.276874600D-12 2.449037044D-16                 -6.021527770D+04-4.479580046D+01
CF3                 Hf:TRC(6/88) w6950. Jacox,1998.
 2 g 8/99 C   1.00F   3.00     0.00     0.00     0.00 0   69.0059096     -467400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11491.470
-2.978307106D+04 7.153678830D+02-3.498185380D+00 3.595457990D-02-4.507974430D-05
 2.821808450D-08-7.098047020D-12                 -6.059997030D+04 4.502592640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11491.470
-2.997305557D+05-1.046989457D+03 1.077923191D+01-3.116087076D-04 6.891351430D-08
-7.911225640D-12 3.670593020D-16                 -5.425304400D+04-3.417038790D+01
CF3+                Chase,1998 p583 12/71. Jacox,1998.
 2 g 9/99 C   1.00F   3.00E  -1.00     0.00     0.00 0   69.0053610      423617.480
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11541.280
-3.587463540D+04 3.743506700D+02 7.787413930D-01 1.929435768D-02-1.892815770D-05
 9.363908760D-09-1.885759656D-12                  4.775581720D+04 2.224044005D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11541.280
-2.910919531D+04-1.996658183D+03 1.144279678D+01-5.653393040D-04 1.232297113D-07
-1.399758046D-11 6.443017950D-16                  5.902345800D+04-4.080349990D+01
CF3Br               Gurvich,1991 pt1 p165 pt2 p144.
 2 tpis91 C   1.00F   3.00BR  1.00     0.00     0.00 0  148.9099096     -648800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14444.028
-5.439489010D+03 1.243615190D+02 9.231941950D-01 3.481044380D-02-4.549645490D-05
 2.932836552D-08-7.548000360D-12                 -8.023396760D+04 2.232999096D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14444.028
-3.834088510D+05-9.719093300D+02 1.372477396D+01-2.901710612D-04 6.421892200D-08
-7.375688770D-12 3.423154250D-16                 -7.765306310D+04-4.717367210D+01
CF3CL               Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p137 pt2 p109.
 2 g 7/99 C   1.00F   3.00CL  1.00     0.00     0.00 0  104.4589096     -704200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13790.751
 1.499409978D+04-1.365768572D+02 1.452912370D+00 3.404765070D-02-4.473777640D-05
 2.888115112D-08-7.434171330D-12                 -8.547166640D+04 1.727327095D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13790.751
-4.066042120D+05-1.022626507D+03 1.376252628D+01-3.052722979D-04 6.755966040D-08
-7.759315250D-12 3.601192290D-16                 -8.410559370D+04-4.913411939D+01
CF4                 Hf:TRC(12/94) w6520. Gurvich,1991 pt1 p79 pt2 p58.
 2 g 7/99 C   1.00F   4.00     0.00     0.00     0.00 0   88.0043128     -933120.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12730.313
 9.817458500D+03 1.163343483D+02-1.288338636D+00 3.959566910D-02-4.996244210D-05
 3.125339346D-08-7.841700320D-12                 -1.138502297D+05 2.938656548D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12730.313
-4.164456780D+05-1.414797167D+03 1.405124837D+01-4.199093860D-04 9.278921610D-08
-1.064575830D-11 4.937099680D-16                 -1.094691149D+05-5.487105000D+01
CH                  Gurvich,1979 pt1 p37 pt2 p39.
 3 tpis79 C   1.00H   1.00     0.00     0.00     0.00 0   13.0186400      597370.604
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8625.104
 2.220590133D+04-3.405411530D+02 5.531452290D+00-5.794964260D-03 7.969554880D-06
-4.465911590D-09 9.596338320D-13                  7.240783270D+04-9.107673050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8625.104
 2.060763440D+06-5.396206660D+03 7.856293850D+00-7.965907450D-04 1.764308305D-07
-1.976386267D-11 5.030429510D-16                  1.062236592D+05-3.154757439D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8625.104
-8.068368690D+08 4.575450540D+05-9.843975080D+01 1.235244098D-02-8.485608570D-07
 3.040410624D-11-4.400315170D-16                 -3.595851590D+06 8.953477440D+02
CH+                 Gurvich,1991 pt1 p38 pt2 p32.
 3 tpis91 C   1.00H   1.00E  -1.00     0.00     0.00 0   13.0180914     1630571.004
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8628.104
 3.019607105D+04-4.618141310D+02 6.225641190D+00-7.775711800D-03 1.094489485D-05
-6.675487910D-09 1.565232409D-12                  1.972491928D+05-1.431512811D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8628.104
-7.102094670D+06 1.828354883D+04-1.312691402D+01 6.191717360D-03-2.909421253D-07
-1.134243575D-10 1.105962085D-14                  7.541296040D+04 1.243984829D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8628.104
-3.160070489D+08 1.436699396D+05-1.108443407D+01 1.562285754D-04 4.928498470D-08
-2.896872362D-12 4.982255990D-17                 -1.013672855D+06 1.489353241D+02
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CHBr3             Kudchadker,1975.
 2 g 8/99 C   1.00H   1.00BR  3.00    0.00    0.00 0  252.7306400      16740.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15906.601
 4.346576860D+04-4.999634420D+02 5.620222110D+00 2.079346321D-02-2.921336328D-05
 2.066942448D-08-5.781220910D-12                 2.627830062D+03 1.247904015D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15906.601
 6.274234950D+05-3.378711100D+03 1.487852612D+01-5.932745270D-04 1.082421577D-07
-1.061012665D-11 4.319152450D-16                 1.877234659D+04-5.311909650D+01
CHCL              Hf:TRC(12/93) w7270.Gurvich,1991. Jacox,1998.
 2 g 9/99 C   1.00H   1.00CL  1.00    0.00    0.00 0   48.4716400     297100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10200.443
-2.699912334D+05 4.351199730D+03-2.275911813D+01 7.550621760D-02-9.071997970D-05
 5.256971860D-08-1.189769182D-11                 1.416862680D+04 1.520980812D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10200.443
-9.548061900D+05 2.174413794D+03 4.867645370D+00 8.321641860D-04-1.536948638D-07
 1.529236537D-11-6.596159360D-16                 1.880121810D+04 2.674761385D+00
CHCLBr2           Gurvich,1991 pt1 p173 pt2 p155.
 2 tpis91 C   1.00H   1.00CL  1.00BR  2.00    0.00 0  208.2796400      10000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15291.236
 3.815380250D+04-4.084175110D+02 4.639244020D+00 2.325990646D-02-3.222988860D-05
 2.254671151D-08-6.256507740D-12                 1.483809044D+03 6.175235281D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15291.236
 6.042865300D+05-3.438241010D+03 1.494162631D+01-6.228427970D-04 1.153724426D-07
-1.147291377D-11 4.733482860D-16                 1.822460958D+04-5.407258924D+01
CHCL2             TRC(12/93) tuvw7270.
 2 n12/93 C   1.00H   1.00CL  2.00    0.00    0.00 0   83.9246400      95800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12800.000
 5.638556130D+04-6.562455420D+02 6.068818020D+00 9.744122600D-03-1.275310131D-05
 8.552386720D-09-2.231582700D-12                 1.330447798D+04-4.533535456D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12800.000
 8.849393710D+05-3.526969730D+03 1.186372153D+01-5.002376120D-04 6.133860400D-08
-1.885433405D-12-1.234221421D-16                 3.071136475D+04-4.088905858D+01
CHCL2Br           Gurvich,1991 pt1 p172 pt2 p154.
 2 tpis91 C   1.00H   1.00CL  2.00BR  1.00    0.00 0  163.8286400     -45000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14729.895
 3.294022650D+04-3.275301170D+02 3.773235240D+00 2.536466143D-02-3.472666990D-05
 2.404666618D-08-6.621730930D-12                -5.425565080D+03 9.433412004D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14729.895
 5.924876440D+05-3.509475610D+03 1.499349593D+01-6.433062570D-04 1.198581809D-07
-1.198476716D-11 4.969948070D-16                 1.197251405D+04-5.602687781D+01
CHCL3             Gurvich,1991 pt1 p127 pt2 p98.
 2 g 7/99 C   1.00H   1.00CL  3.00    0.00    0.00 0  119.3776400    -102700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14305.494
 3.395333290D+04-3.047428785D+02 2.923672263D+00 2.830547858D-02-3.712424690D-05
 2.551365915D-08-6.987659550D-12                -1.235063157D+04 1.115556408D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14305.494
 6.136052740D+05-3.715087170D+03 1.510777247D+01 2.362584336D-04 1.297140438D-07
-1.267494791D-11 5.259022310D-16                 6.203313450D+03-5.992576539D+01
CHF               Hf:TRC(6/88) w695. Jacox,1998.
 2 g 8/99 C   1.00H   1.00F   1.00    0.00    0.00 0   32.0170432     108800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9981.216
-7.868585830D+04 1.300218466D+03-3.947685250D+00 2.114995848D-02-2.239962738D-05
 1.283155181D-08-2.904778136D-12                 5.824389720D+03 4.785453770D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9981.216
 3.994085420D+06-7.962756200D+03 6.755595090D+00 4.949836570D-03-2.101763812D-06
 3.348232950D-10-1.886825050D-14                 6.706134940D+04-2.381240379D+01
CHFBr2            Gurvich,1991 pt1 p168 pt2 p149.
 2 tpis91 C   1.00H   1.00F   1.00BR  2.00    0.00 0  191.8250432    -175000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14359.556
-1.820197980D+04 4.362249670D+02-3.733854170D-01 3.388631400D-02-4.371298530D-05
 2.889569295D-08-7.683915110D-12                -2.465611586D+04 3.320478790D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14359.556
 5.935751630D+05-3.742656580D+03 1.517184031D+01-7.158039030D-04 1.360636972D-07
-1.385897355D-11 5.844209110D-16                -2.347676027D+03-5.765783430D+01
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CHFCL             Gurvich,1991 pt1 p147 pt2 p121.
 2 tpis91 C   1.00H   1.00F   1.00CL  1.00     0.00 0   67.4700432     -83144.704
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11145.955
-7.113008510D+04 1.377872745D+03-6.484617240D+00 3.890972490D-02-4.800735220D-05
 3.073300019D-08-7.982853410D-12                 -1.751793745D+04 6.373895867D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11145.955
 6.622163580D+05-3.809007980D+03 1.223880469D+01-7.467182750D-04 1.434767850D-07
-1.475406631D-11 6.273780680D-16                  1.018987746D+04-4.658365563D+01
CHFCLBr           Gurvich,1991 pt1 p176 pt2 p159.
 2 tpis91 C   1.00H   1.00F   1.00CL  1.00BR  1.00 0  147.3740432     -230000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13787.186
-1.959240614D+04 4.901723270D+02-1.259408503D+00 3.617708470D-02-4.654244960D-05
 3.065240659D-08-8.123903600D-12                 -3.139900705D+04 3.710450945D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13787.186
 5.800117510D+05-3.823337850D+03 1.522809062D+01-7.373906310D-04 1.407097155D-07
-1.438245319D-11 6.083867150D-16                 -8.552249900D+03-5.903677705D+01
CHFCL2            Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p149 pt2 p124.
 2 g 7/99 C   1.00H   1.00F   1.00CL  2.00     0.00 0  102.9230432     -284900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13294.362
-1.734959015D+04 4.924913200D+02-1.854635884D+00 3.782786280D-02-4.863343040D-05
 3.197197630D-08-8.459057990D-12                 -3.788749270D+04 3.801530544D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13294.362
 5.640113020D+05-3.887083300D+03 1.527760246D+01-7.576487420D-04 1.452498792D-07
-1.490796515D-11 6.328998500D-16                 -1.484736185D+04-6.167535516D+01
CHF2              TRC(6/88) tuvw6950.
 2 n 6/88 C   1.00H   1.00F   2.00     0.00     0.00 0   51.0154464     -238900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10920.000
-1.469690117D+05 2.553397313D+03-1.302627630D+01 5.438128460D-02-6.713418790D-05
 4.287651730D-08-1.110824216D-11                 -4.179372160D+04 9.939930250D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10920.000
 5.526806550D+05-3.696009170D+03 1.208610573D+01-6.498588100D-04 1.120846220D-07
-9.814147010D-12 3.349192390D-16                 -9.437068420D+03-4.704416200D+01
CHF2Br            Gurvich,1991 pt1 p168 pt2 p148.
 2 tpis91 C   1.00H   1.00F   2.00BR  1.00     0.00 0  130.9194464     -422000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13169.504
-7.714510160D+04 1.422544046D+03-6.684393650D+00 4.738389150D-02-5.830588750D-05
 3.695720470D-08-9.495485280D-12                 -5.878500930D+04 6.608639090D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13169.504
 5.767706840D+05-4.177716080D+03 1.550150581D+01-8.490147290D-04 1.657177491D-07
-1.727828054D-11 7.435627230D-16                 -2.966147348D+04-6.349380140D+01
CHF2CL            Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p148 pt2 p123.
 2 g 7/99 C   1.00H   1.00F   2.00CL  1.00     0.00 0   86.4684464     -482800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12367.496
-7.240579410D+04 1.365510973D+03-7.153222080D+00 4.854987970D-02-5.948781670D-05
 3.750966190D-08-9.589524420D-12                 -6.565932800D+04 6.657212230D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12367.496
 5.629493730D+05-4.298673050D+03 1.558191398D+01-8.789278480D-04 1.720248689D-07
-1.797910869D-11 7.753391700D-16                 -3.634067160D+04-6.611261480D+01
CHF3              Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p97 pt2 p72.
 2 g 8/99 C   1.00H   1.00F   3.00     0.00     0.00 0   70.0138496     -693300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11566.886
-1.095132260D+05 2.042273879D+03-1.166213079D+01 5.785807770D-02-6.857135060D-05
 4.212118380D-08-1.053196888D-11                 -9.395470050D+04 8.935920650D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11566.886
 5.685232020D+05-4.728361700D+03 1.586728516D+01-7.382348650D-04 1.970841706D-07
-2.062115571D-11 8.970599640D-16                 -5.923196370D+04-7.161273220D+01
CHI3              Kudchadker,1975.
 2 g 8/99 C   1.00H   1.00I   3.00     0.00     0.00 0  393.7320500     210873.600
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17156.587
 5.252923590D+04-7.242166470D+02 8.018623340D+00 1.470995487D-02-2.163843469D-05
 1.594571452D-08-4.601437960D-12                  2.678186915D+04-8.605054840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17156.587
 6.294205430D+05-3.184061570D+03 1.479622178D+01-5.749555500D-04 1.062025541D-07
-1.052804696D-11 4.329720020D-16                  4.103609800D+04-4.901357390D+01
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CH2              D0(H2C-H): Ruscic,1999. Jacox,1998.
 2 g 4/02 C   1.00H   2.00    0.00    0.00    0.00 0   14.0265800     390364.517
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10027.417
 3.218921730D+04-2.877601815D+02 4.203583820D+00 3.455405960D-03-6.746193340D-06
 7.654571640D-09-2.870328419D-12 0.000000000D+00 4.733624710D+04-2.143628603D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10027.417
 2.550418031D+06-7.971625390D+03 1.228924487D+01-1.699122922D-03 2.991728605D-07
-2.767007492D-11 1.051341740D-15 0.000000000D+00 9.642216890D+04-6.094739910D+01
CH2Br2           Kudchadker, 1975.
 2 g 8/99 C   1.00H   2.00BR  2.00    0.00    0.00 0  173.8345800     -14770.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12614.407
 4.797308010D+03 3.613859240D+02-1.819592338D+00 3.477048340D-02-4.498546180D-05
 3.068623685D-08-8.434846340D-12               -4.481497060D+03 3.827123590D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12614.407
 1.528284441D+06-6.673414950D+03 1.670213316D+01-1.166351237D-03 2.122634493D-07
-2.075472240D-11 8.428577700D-16               3.600706640D+04-7.448065490D+01
CH2CL            Hf:TRC(12/93) w7270. Gurvich,1991 pt1 p122. Jacox,1998.
 2 g12/99 C   1.00H   2.00CL  1.00    0.00    0.00 0   49.4795800     119200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10979.920
-3.188585630D+04 6.333163210D+02-1.164065495D+00 2.160586080D-02-2.545462163D-05
 1.693887757D-08-4.660078600D-12               1.020142540D+04 3.230835289D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10979.920
 1.662438334D+06-6.441125720D+03 1.359753722D+01-1.140536810D-03 2.087760159D-07
-2.052347186D-11 8.375772270D-16               5.212906120D+04-6.148586271D+01
CH2CLBr          Gurvich,1991 pt1 p171 pt2 p153.
 2 tpis91 C   1.00H   2.00CL  1.00BR  1.00    0.00 0  129.3835800     -45000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12190.747
-1.307948755D+04 6.455860380D+02-3.577349910D+00 3.833687230D-02-4.864252050D-05
 3.261622330D-08-8.852877390D-12               -9.402272530D+03 4.748806758D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12190.747
 1.525016309D+06-6.823334160D+03 1.682769102D+01-1.219735119D-03 2.244964495D-07
-2.219063248D-11 9.104705130D-16               3.320239920D+04-7.637571062D+01
CH2CL2           Gurvich,1991 pt1 p125 pt2 p97.
 2 tpis91 C   1.00H   2.00CL  2.00    0.00    0.00 0   84.9325800     -95000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11854.077
-2.509841179D+04 8.687667380D+02-5.094669210D+00 4.150049990D-02-5.199772150D-05
 3.445944260D-08-9.270292520D-12               -1.638978840D+04 5.396890320D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11854.077
 1.529279337D+06-6.976954760D+03 1.694154931D+01-1.265053995D-03 2.344766734D-07
-2.333227421D-11 9.632834730D-16               2.806318171D+04-7.949453510D+01
CH2F             TRC(6/88) tuvw6950.
 2 n 6/88 C   1.00H   2.00F   1.00    0.00    0.00 0   33.0249832     -31800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11129.000
-8.569712530D+04 1.392226749D+03-4.382052590D+00 2.645916948D-02-2.848145663D-05
 1.732706028D-08-4.442061440D-12               -1.169444586D+04 5.049499200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11129.000
 2.535399502D+06-9.358439020D+03 1.700366206D+01-3.062919929D-03 7.612869080D-07
-9.664554980D-11 4.844768100D-15               5.228391310D+04-8.707551570D+01
CH2FBr           Gurvich,1991 pt1 p167 pt2 p147.
 2 tpis91 C   1.00H   2.00F   1.00BR  1.00    0.00 0  112.9289832    -215000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11622.586
-9.256109530D+04 1.811985865D+03-9.698346870D+00 5.035848670D-02-6.070272680D-05
 3.878250800D-08-1.012615992D-11               -3.537509620D+04 8.140396050D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11622.586
 1.539975462D+06-7.231551360D+03 1.714566439D+01-1.350184394D-03 2.538022824D-07
-2.558977386D-11 1.069310946D-15               1.509604224D+04-8.062053710D+01
CH2FCL           Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p147 pt2 p122.
 2 g 7/99 C   1.00H   2.00F   1.00CL  1.00    0.00 0   68.4779832     -265700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11252.357
-1.071340332D+05 2.081328396D+03-1.155723697D+01 5.441482110D-02-6.518622740D-05
 4.133159880D-08-1.071935103D-11               -4.264756210D+04 9.035923547D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11252.357
 1.536120418D+06-7.378939730D+03 1.725797178D+01-1.395645457D-03 2.639247747D-07
-2.675653563D-11 1.123582778D-15               9.813710460D+03-8.313642553D+01
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Appendix D (*continued*)

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CH2F2             Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p96 pt2 p71.
 2 g 8/99 C   1.00H   2.00F   2.00    0.00    0.00 0   52.0233864    -452300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10693.327
-1.819917500D+05 3.174427890D+03-1.714256906D+01 6.411353830D-02-7.313592120D-05
 4.426384160D-08-1.103877216D-11                -7.027058950D+04 1.207331926D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10693.327
 1.546609496D+06-7.876883330D+03 1.768770469D+01-1.581298721D-03 3.068917255D-07
-3.183405460D-11 1.363827177D-15                -9.800135960D+03-8.907420360D+01
CH2I2             Kudchadker,1975. Kudchadker,1976.
 2 g 8/99 C   1.00H   2.00I   2.00    0.00    0.00 0  267.8355200     117570.400
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13250.428
 2.738133757D+04-8.972568040D+01 1.387869408D+00 2.733482611D-02-3.619408770D-05
 2.539187610D-08-7.145585160D-12                 1.338767276D+04 2.241870165D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13250.428
 1.512892716D+06-6.442912400D+03 1.659026137D+01-1.135551520D-03 2.073750250D-07
-2.033902231D-11 8.282283700D-16                 5.058219030D+04-7.125235140D+01
CH3               D0(H3C-H): Ruscic,1999. Jacox,1998.
 2 g 4/02 C   1.00H   3.00    0.00    0.00    0.00 0   15.0345200     146658.040
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10366.340
-2.876188806D+04 5.093268660D+02 2.002143949D-01 1.363605829D-02-1.433989346D-05
 1.013556725D-08-3.027331936D-12 0.000000000D+00 1.408271825D+04 2.022772791D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10366.340
 2.760802663D+06-9.336531170D+03 1.487729606D+01-1.439429774D-03 2.444477951D-07
-2.224555778D-11 8.395065760D-16 0.000000000D+00 7.481809480D+04-7.919682400D+01
CH3Br             Kudchadker,1975.
 2 g 8/99 C   1.00H   3.00BR  1.00    0.00    0.00 0   94.9385200     -37740.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10612.655
-7.115585770D+04 1.524705928D+03-8.230445210D+00 4.239973210D-02-4.946979890D-05
 3.194433340D-08-8.531237080D-12                -1.251753591D+04 7.048127770D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10612.655
 2.524874348D+06-1.011876098D+04 1.865902163D+01-1.797673690D-03 3.298520110D-07
-3.250912030D-11 1.330179925D-15                 5.540576390D+04-9.778664460D+01
CH3CL             Gurvich,1991 pt1 p122 pt2 p95.
 2 tpis91 C   1.00H   3.00CL  1.00    0.00    0.00 0   50.4875200     -81870.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10416.144
-9.841971100D+04 1.983700841D+03-1.084512305D+01 4.777980050D-02-5.515516260D-05
 3.506176140D-08-9.236103960D-12                -1.994689506D+04 8.399658331D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10416.144
 2.522463305D+06-1.030115447D+04 1.882725852D+01-1.872291294D-03 3.473372860D-07
-3.458887220D-11 1.428941079D-15                 5.111417410D+04-1.006571389D+02
CH3F              Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p93 pt2 p69.
 2 g 8/99 C   1.00H   3.00F   1.00    0.00    0.00 0   34.0329232    -237700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10135.229
-2.029821878D+05 3.447331130D+03-1.768994275D+01 5.945275800D-02-6.469528250D-05
 3.859418040D-08-9.626541530D-12                -4.577926220D+04 1.228382176D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10135.229
 2.561903188D+06-1.086052758D+04 1.929446920D+01-2.070973131D-03 3.929124530D-07
-3.994503420D-11 1.681447081D-15                 3.563508510D+04-1.061158456D+02
CH3I              Kudchadker,1975.
 2 g 8/99 C   1.00H   3.00I   1.00    0.00    0.00 0  141.9389900     13765.360
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10815.834
-4.516462740D+04 1.086208429D+03-5.663176270D+00 3.683171710D-02-4.321393500D-05
 2.833483666D-08-7.684383690D-12                -4.303830650D+03 5.688562690D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10815.834
 2.511915982D+06-9.960289990D+03 1.856907132D+01-1.768191331D-03 3.242206260D-07
-3.192942010D-11 1.305407821D-15                 6.066929950D+04-9.590777040D+01
CH2OH             Hydroxymethyl Radical. Johnson,1996.
 2 g11/00 C   1.00H   3.00O   1.00    0.00    0.00 0   31.0339200     -17800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11781.000
-1.560076238D+05 2.685446279D+03-1.342022420D+01 5.757139470D-02-7.284449990D-05
 4.836648860D-08-1.293492601D-11                -1.596820410D+04 9.963033700D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11781.000
 2.250349506D+06-8.173186060D+03 1.599639179D+01-8.704133720D-04 6.069183950D-08
 4.408349460D-12-5.702309500D-16                 4.645313430D+04-7.835158450D+01
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CH2OH+            Hydroxymethyl Cation. Johnson,1996.
 2 g11/00 C   1.00H   3.00O   1.00E  -1.00    0.00 0   31.0333714     716400.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10149.000
-1.077080841D+05 2.252082711D+03-1.188167865D+01 4.602316960D-02-4.879736880D-05
 2.876413471D-08-7.100226500D-12                 7.484447770D+04 9.027928570D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10149.000
 2.603333487D+06-1.009953810D+04 1.730843898D+01-6.946390320D-04 3.009715083D-08
 5.221485980D-12-5.090183790D-16                 1.465402426D+05-9.223955280D+01
CH3O              Hf:Gurvich,1991 pt1 p67. Jacox,1998 p271.
 2 g 7/00 C   1.00H   3.00O   1.00    0.00    0.00 0   31.0339200     13000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11302.050
 8.657117660D+04-6.631685250D+02 2.257455672D+00 2.266283789D-02-2.970566403D-05
 2.199341353D-08-6.588043380D-12                 4.174102130D+03 8.174777900D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11302.050
 2.101188243D+06-8.841968800D+03 1.822645731D+01-1.743485034D-03 3.340434270D-07
-3.430673160D-11 1.473897771D-15                 5.309582060D+04-9.422500590D+01
CH4               Gurvich,1991 pt1 p44 pt2 p36.
 2 g 8/99 C   1.00H   4.00    0.00    0.00    0.00 0   16.0424600     -74600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10016.202
-1.766850998D+05 2.786181020D+03-1.202577850D+01 3.917619290D-02-3.619054430D-05
 2.026853043D-08-4.976705490D-12                -2.331314360D+04 8.904322750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10016.202
 3.730042760D+06-1.383501485D+04 2.049107091D+01-1.961974759D-03 4.727313040D-07
-3.728814690D-11 1.623737207D-15                 7.532066910D+04-1.219124889D+02
CH3OH             Hf:TRC(6/87) w5030. Chen,1977.
 2 g 7/00 C   1.00H   4.00O   1.00    0.00    0.00 0   32.0418600    -200940.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11435.277
-2.416642886D+05 4.032147190D+03-2.046415436D+01 6.903698070D-02-7.598932690D-05
 4.598208360D-08-1.158706744D-11                -4.433261170D+04 1.400142190D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11435.277
 3.411570760D+06-1.345500201D+04 2.261407623D+01-2.141029179D-03 3.730050540D-07
-3.498846390D-11 1.366073444D-15                 5.636081560D+04-1.277814279D+02
CH3OOH            Methyl Hydroperoxide, CH3-O-O-H. Dorofeeva,2001.
 2 srd 01 C   1.00H   4.00O   2.00    0.00    0.00 0   48.0412600    -139000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13918.692
-1.497974156D+05 2.656222273D+03-1.377060625D+01 6.588673830D-02-7.751801650D-05
 4.968800700D-08-1.314367640D-11 0.000000000D+00-3.058414201D+04 1.031696850D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13918.692
 3.060740610D+06-1.282959627D+04 2.541021168D+01-2.394481095D-03 4.443429910D-07
-4.416659500D-11 1.819673372D-15 0.000000000D+00 5.837492360D+04-1.387713096D+02
CI                Gurvich,1991 pt1 p176 pt2 p160.
 2 tpis91 C   1.00I   1.00    0.00    0.00    0.00 0  138.9151700     570200.814
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9494.114
 1.043011064D+05-1.715427168D+03 1.288874952D+01-1.828504834D-02 2.135468356D-05
-1.286980869D-08 3.167047660D-12                 7.550784700D+04-4.496811320D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9494.114
-2.408229894D+05 3.447387040D+02 4.976968700D+00-8.444815390D-04 5.061239720D-07
-1.047700525D-10 6.740843140D-15                 6.451342020D+04 1.090913159D+00
CI2               Gurvich,1991 pt1 p178 pt2 p161.
 2 tpis91 C   1.00I   2.00    0.00    0.00    0.00 0  265.8196400     468393.633
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12643.133
 6.028289810D+04-1.043205435D+03 1.017465942D+01-5.535671710D-03 5.630319010D-06
-3.108249657D-09 7.202469560D-13                 5.964896550D+04-2.310319208D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12643.133
-7.028655530D+05 3.082750393D+02 9.046427050D+00-2.946736644D-03 1.424347233D-06
-2.453183410D-10 1.425270291D-14                 5.021134210D+04-1.560349377D+01
CI3               Gurvich,1991 pt1 p178 pt2 p162.
 2 g 9/99 C   1.00I   3.00    0.00    0.00    0.00 0  392.7241100     405983.951
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16831.451
 8.596784250D+04-1.347703793D+03 1.272103659D+01-2.442876357D-03 2.511609978D-07
 1.024658583D-09-4.872692960D-13                 5.310716510D+04-3.238492900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16831.451
-1.536511918D+05-8.357044370D+01 1.006203125D+01-2.466447336D-05 5.419054750D-09
-6.181417000D-13 2.851262022D-17                 4.582589530D+04-1.494825345D+01
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CI4                Kudchadker,1975. Kudchadker,1976.
 2 g 8/99 C   1.00I   4.00    0.00    0.00    0.00 0  519.6285800     267943.360
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22355.550
 8.919043870D+04-1.651906475D+03 1.796124325D+01-8.518114250D-03 8.508682250D-06
-4.599097730D-09 1.039492403D-12                 3.689392150D+04-5.805953120D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22355.550
-1.446762770D+05-5.280365170D+01 1.303985589D+01-1.606214814D-05 3.567550470D-09
-4.105366980D-13 1.907272766D-17                 2.817746618D+04-2.810414436D+01
CN                 Hf: Huang,1992. Gurvich,1979 pt1 p212 pt2 p210.
 3 g 8/99 C   1.00N   1.00    0.00    0.00    0.00 0   26.0174000     438683.552
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8672.104
 3.949148570D+03-1.391590572D+02 4.930835320D+00-6.304670510D-03 1.256836472D-05
-9.878300500D-09 2.843137221D-12                 5.228455380D+04-2.763115585D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8672.104
-2.228006270D+06 5.040733390D+03-2.121897722D-01 1.354901134D-03 1.325929798D-07
-6.937006370D-11 5.494952270D-15                 1.784496132D+04 3.282563919D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8672.104
-1.794798118D+08 1.054346069D+05-1.729624170D+01 2.194895530D-03-8.508938030D-08
 9.318692990D-13 6.358139930D-18                -7.962594120D+05 1.913139639D+02
CN+                Gurvich,1991 pt1 p215 pt2 p203.
 3 tpis91 C   1.00N   1.00E -1.00    0.00    0.00 0   26.0168514    1798890.904
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8682.104
-8.302909570D+05 8.775687500D+03-2.977443560D+01 4.976897060D-02-1.302225951D-05
-2.058325353D-08 1.126843895D-11                 1.703860539D+05 2.039918818D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8682.104
-7.153463080D+06 1.857250421D+04-1.084534159D+01 6.106681430D-03-1.191208566D-06
 1.184848778D-10-4.799838730D-15                 9.242644960D+04 1.135340573D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8682.104
-2.354919695D+08 1.433776703D+05-2.975360271D+01 4.280545600D-03-2.707260413D-07
 8.178340660D-12-9.629506200D-17                -9.229047140D+05 2.964624987D+02
CN-                Gurvich,1991 pt1 p218 pt2 p205.
 2 tpis91 C   1.00N   1.00E   1.00    0.00    0.00 0   26.0179486      63885.104
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
-4.606541390D+04 4.294174750D+02 2.328781880D+00-1.235303004D-04 4.478462770D-06
-4.403151290D-09 1.349001191D-12                 4.362078340D+03 1.142928617D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 3.517964720D+05-1.630477359D+03 5.609875750D+00-3.975605970D-04 8.856147080D-08
-9.722872320D-12 4.434205690D-16                 1.647976581D+04-1.175502699D+01
CNN                Gurvich,1991 pt1 p220 pt2 p208. Jacox,1994.
 2 g12/99 C   1.00N   2.00    0.00    0.00    0.00 0   40.0241000     633484.056
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10377.660
-7.357692360D+04 9.652438660D+02-1.704121157D+00 2.037239025D-02-2.183423906D-05
 1.176082777D-08-2.551355221D-12                 7.021729830D+04 3.528150910D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10377.660
-1.817148765D+05-6.729863490D+02 7.857948340D+00-6.136880720D-05-1.088178985D-08
 4.456655810D-12-2.836496278D-16                 7.723488980D+04-1.966012324D+01
CO                 Gurvich,1979 pt1 p25 pt2 p29.
 3 tpis79 C   1.00O   1.00    0.00    0.00    0.00 0   28.0101000    -110535.196
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 1.489045326D+04-2.922285939D+02 5.724527170D+00-8.176235030D-03 1.456903469D-05
-1.087746302D-08 3.027941827D-12                -1.303131878D+04-7.859241350D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 4.619197250D+05-1.944704863D+03 5.916714180D+00-5.664282830D-04 1.398814540D-07
-1.787680361D-11 9.620935570D-16                -2.466261084D+03-1.387413108D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 8.868662960D+08-7.500377840D+05 2.495474979D+02-3.956351100D-02 3.297772080D-06
-1.318409933D-10 1.998937948D-15                 5.701421130D+06-2.060704786D+03
CO+                Gurvich,1991 pt1 p26 pt2 p22.
 3 tpis91 C   1.00O   1.00E -1.00    0.00    0.00 0   28.0095514    1247789.204
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
-2.178786658D+04 1.288857032D+02 3.769057550D+00-3.431730130D-03 8.193945750D-06
-6.463814690D-09 1.803727574D-12                 1.482345898D+05 3.990547070D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 2.316847506D+05-1.057646148D+03 4.554257780D+00 4.495520320D-04-2.489507047D-07
 5.267566420D-11-3.289510270D-15                 1.555050724D+05-3.873462640D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
-3.035604054D+08 2.393118392D+05-7.034999240D+01 1.139551440D-02-8.315173100D-07
 2.863705515D-11-3.803269410D-16                -1.688617704D+06 6.291980420D+02
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Appendix D (*continued*)

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COCL              Gurvich,1991 pt1 p118 pt2 p91.
 2 tpis91 C   1.00O   1.00CL  1.00     0.00     0.00 0   63.4631000     -16000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11550.749
 2.513175740D+04-5.969189670D+02 8.327671350D+00-7.056132590D-03 1.313150734D-05
-1.037059653D-08 3.033665179D-12                 -7.052770320D+02-1.580716775D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11550.749
 3.443720240D+05-1.793143470D+03 8.392755900D+00-5.374769590D-04 9.113555710D-08
-3.111441728D-12-2.040435218D-16                  6.914470150D+03-1.998919104D+01
COCL2             Gurvich,1991 pt1 p119 pt2 p92.
 2 tpis91 C   1.00O   1.00CL  2.00     0.00     0.00 0   98.9161000     -219500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12878.622
 9.319321450D+04-1.577971273D+03 1.208353907D+01-4.809015610D-03 7.688477320D-06
-5.858841200D-09 1.687786559D-12                 -2.054252334D+04-3.834767320D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12878.622
-2.545881891D+04-1.305958516D+03 1.092922584D+01-3.601210160D-04 7.787017650D-08
-8.792452030D-12 4.028696610D-16                 -2.219847340D+04-3.233303450D+01
COFCL             Gurvich,1991 pt1 p146 pt2 p120.
 2 tpis91 C   1.00O   1.00F   1.00CL  1.00     0.00 0   82.4615032     -429492.862
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11903.798
 7.262173900D+04-1.019738175D+03 7.290911990D+00 7.420691710D-03-7.902548080D-06
 4.209427650D-09-9.314412900D-13                 -4.804386460D+04-1.316923671D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11903.798
-5.316887910D+04-1.581009678D+03 1.112696501D+01-4.373000800D-04 9.464190710D-08
-1.069291346D-11 4.901756640D-16                 -4.599667230D+04-3.525879824D+01
COF2              Gurvich,1991 pt1 p89 pt2 p66.
 2 tpis91 C   1.00O   1.00F   2.00     0.00     0.00 0   66.0069064     -640000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11133.929
 5.263393150D+04-4.618603390D+02 2.774114516D+00 1.831931082D-02-2.130172554D-05
 1.266924542D-08-3.101675983D-12                 -7.564255100D+04 9.467181460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11133.929
-4.073806850D+04-1.974009812D+03 1.140363654D+01-5.437111470D-04 1.175232744D-07
-1.326564192D-11 6.076772130D-16                 -6.907795410D+04-4.009695000D+01
COHCL             Gurvich,1991 pt1 p134 pt2 p106.
 2 tpis91 C   1.00O   1.00H   1.00CL  1.00     0.00 0   64.4710400     -164211.876
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11006.282
 6.332946870D+03 8.120365590D+01 1.374648391D+00 1.650970564D-02-1.692917241D-05
 9.684046830D-09-2.374469390D-12                 -2.120356580D+04 1.938379650D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11006.282
 8.318952850D+05-4.416870840D+03 1.270661114D+01-9.361408630D-04 1.855335611D-07
-1.958378539D-11 8.512046830D-16                  4.330496440D+03-5.145071542D+01
COHF              Gurvich,1991 pt1 p106 pt2 p80.
 2 tpis91 C   1.00O   1.00H   1.00F   1.00     0.00 0   48.0164432     -374590.361
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10449.795
-4.585828500D+04 1.048202675D+03-4.776574220D+00 3.080719931D-02-3.415895900D-05
 2.034926806D-08-5.054194620D-12                 -5.085983730D+04 5.232247410D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10449.795
 8.578853160D+05-4.791959120D+03 1.293975218D+01-1.018285299D-03 2.021278474D-07
-2.136698091D-11 9.299588910D-16                 -1.878933107D+04-5.527449140D+01
COS               Gurvich,1991 pt1 p211 pt2 p200.
 2 g 5/01 C   1.00O   1.00S   1.00     0.00     0.00 0   60.0751000     -141700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9941.597
 8.547876430D+04-1.319464821D+03 9.735257240D+00-6.870830960D-03 1.082331416D-05
-7.705597340D-09 2.078570344D-12                 -1.191657685D+04-2.991988593D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9941.597
 1.959098567D+05-1.756167688D+03 8.710430340D+00-4.139424960D-04 1.015243648D-07
-1.159609663D-11 5.691053860D-16                 -8.927096690D+03-2.636328016D+01
CO2               Gurvich,1991 pt1 p27 pt2 p24.
 3 g 9/99 C   1.00O   2.00     0.00     0.00     0.00 0   44.0095000     -393510.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9365.469
 4.943650540D+04-6.264116010D+02 5.301725240D+00 2.503813816D-03-2.127308728D-07
-7.689988780D-10 2.849677801D-13                 -4.528198460D+04-7.048279440D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9365.469
 1.176962419D+05-1.788791477D+03 8.291523190D+00-9.223156780D-05 4.863676880D-09
-1.891053312D-12 6.330036590D-16                 -3.908350590D+04-2.652669281D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9365.469
-1.544423287D+09 1.016847056D+06-2.561405230D+02 3.369401080D-02-2.181184337D-06
 6.991420840D-11-8.842351500D-16                 -8.043214510D+06 2.254177493D+03
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CO2+              Gurvich,1991 pt1 p30 pt2 p26.
 3 g 9/99 C   1.00O   2.00E  -1.00     0.00     0.00 0   44.0089514     944687.989
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10566.089
-7.383030980D+04 1.086211742D+03-2.771112737D+00 2.318463595D-02-2.570240315D-05
 1.450335497D-08-3.334470420D-12                  1.071784918D+05 4.054885210D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10566.089
-1.695051682D+05-8.066469730D+02 8.002828460D+00-1.577214041D-04 2.566759314D-08
-2.404195965D-12 1.677446800D-16                  1.154389478D+05-2.133567772D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10566.089
-8.365409060D+07 5.333327510D+04-5.621698360D+00 1.491439440D-03-7.553254510D-08
 1.794658103D-12-1.627521598D-17                 -3.111917656D+05 9.673884890D+01
COOH              Gurvich,1991 pt1 p60 pt2 p46.
 2 tpis91 C   1.00O   2.00H   1.00     0.00     0.00 0   45.0174400    -213000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10813.349
-1.128380671D+04 3.775179430D+02-5.992550410D-01 2.181894272D-02-2.425918417D-05
 1.451245206D-08-3.596233380D-12                 -2.841042565D+04 2.934561769D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10813.349
 9.293188730D+05-4.483030570D+03 1.242199567D+01-7.463139640D-04 1.332996131D-07
-1.282710550D-11 5.137997900D-16                 -8.518232680D+02-5.068065510D+01
CP                Gurvich,1991 pt1 p231 pt2 p219.
 2 tpis91 C   1.00P   1.00    0.00     0.00     0.00 0   42.9844610     520161.805
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8715.105
-4.523940110D+04 7.758828140D+02-1.453947907D+00 1.397713706D-02-1.624489706D-05
 9.514083880D-09-2.210281109D-12                  5.792634670D+04 3.311647920D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8715.105
-5.449937150D+06 1.688345926D+04-1.595692200D+01 1.136028761D-02-2.846541330D-06
 3.379364040D-10-1.554457397D-14                 -4.554517740D+04 1.451324059D+02
CS                Hf:Prinslow,1991. Gurvich,1991 pt1 p206 pt2 p198.
 2 g11/01 C   1.00S   1.00    0.00     0.00     0.00 0   44.0757000     278550.078
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8708.378
-4.924844120D+04 8.166968100D+02-1.542998408D+00 1.380324735D-02-1.574407905D-05
 9.169714930D-09-2.169700595D-12                  2.865182876D+04 3.308541327D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8708.378
-9.719574760D+05 2.339201284D+03 1.709390402D+00 1.577178949D-03-4.146335910D-07
 4.504757080D-11-5.945457730D-16                  1.681020727D+04 1.874048220D+01
CS2               Gurvich,1991 pt1 p209 pt2 p199.
 2 g 6/95 C   1.00S   2.00    0.00     0.00     0.00 0   76.1407000     116700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10664.223
 1.613560482D+04-4.649481470D+02 6.297938790D+00 1.888896706D-03 3.031927747D-07
-1.737645373D-09 7.793989390D-13                  1.477761119D+04-9.303382130D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10664.223
-1.390419724D+06 3.354975500D+03 3.019247723D+00 2.876437543D-03-9.076812720D-07
 1.374091042D-10-6.999575570D-15                 -1.013898046D+04 1.565113703D+01
C2                Gurvich,1991 pt1 p9 pt2 p8.
 3 tpis91 C   2.00    0.00    0.00     0.00     0.00 0   24.0214000     830457.322
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10169.122
 5.559634510D+05-9.980126440D+03 6.681620370D+01-1.743432724D-01 2.448523051D-04
-1.703467580D-07 4.684527730D-11                  1.445869634D+05-3.448229700D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10169.122
-9.689267930D+05 3.561092990D+03-5.064138930D-01 2.945154879D-03-7.139441190D-07
 8.670657250D-11-4.076906810D-15                  7.681796830D+04 3.339985240D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10169.122
 6.315145920D+06 1.365420661D+04-3.996903670D+00 1.937561376D-03-1.584446580D-07
 5.520861660D-12-7.253735340D-17                  9.387024990D+03 6.614329920D+01
C2+               Gurvich,1991 pt1 p14 pt2 p10.
 3 tpis91 C   2.00E  -1.00    0.00     0.00     0.00 0   24.0208514    2004775.532
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8685.104
-9.913423840D+04 1.347170609D+03-3.476753160D+00 1.676429424D-02-1.865908025D-05
 1.091134647D-08-2.434913818D-12                  2.335454800D+05 4.406644620D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8685.104
 3.836292810D+06-6.242062450D+03 2.779245639D+00 6.065865860D-03-2.452799858D-06
 3.882942500D-10-2.190639912D-14                  2.857447553D+05 7.297383490D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8685.104
 4.992689800D+07-2.017309121D+04 6.342227540D+00 6.369922600D-04-1.036760828D-07
 4.943272920D-12-7.988804260D-17                  4.120857610D+05-2.112967169D+01
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C2-                Gurvich,1991 pt1 p15 pt2 p12.
 2 tpis91 C   2.00E   1.00     0.00     0.00     0.00 0   24.0219486      480766.904
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8676.104
-1.181928660D+05 1.438189710D+03-3.196131350D+00 1.465548163D-02-1.545537278D-05
 9.061235610D-09-2.135962274D-12                 4.965317790D+04 4.225608880D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8676.104
 4.478136250D+06-1.154145714D+04 1.310143499D+01-1.862700578D-03 4.006931250D-08
 3.710213600D-11-3.337266870D-15                 1.325356168D+05-6.975964400D+01
C2CL               Gurvich,1991 pt1 p112 pt2 p85.
 2 tpis91 C   2.00CL  1.00     0.00     0.00     0.00 0   59.4744000      534083.071
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10780.626
 4.725889410D+04-8.980223610D+02 9.016877150D+00-6.333782830D-03 1.087060050D-05
-8.089068920D-09 2.248275223D-12                 6.702215700D+04-2.354893403D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10780.626
 2.137368408D+05-1.630519518D+03 8.623490250D+00-4.253517860D-04 9.040018640D-08
-1.007541495D-11 4.570764750D-16                 7.171093280D+04-2.413014598D+01
C2CL2              Hf:Manion,2002. Gurvich,1991 pt1 p114 pt2 p86.
 2 g 5/02 C   2.00CL  2.00     0.00     0.00     0.00 0   94.9268000      226600.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14592.612
 3.871169080D+04-9.336870730D+02 1.119377861D+01-3.746288200D-03 6.770472560D-06
-4.910388350D-09 1.299068749D-12 0.000000000D+00 2.948153198D+04-3.310724640D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14592.612
 2.961978472D+05-2.044286552D+03 1.187529315D+01-5.115011450D-04 1.072661556D-07
-1.183411171D-11 5.326498340D-16 0.000000000D+00 3.636799690D+04-4.000823970D+01
C2CL3              Gurvich,1991 pt1 p114 pt2 p87.
 2 tpis91 C   2.00CL  3.00     0.00     0.00     0.00 0  130.3804000      190271.592
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16150.258
 4.675016040D+04-8.851019640D+02 9.032270550D+00 1.242122796D-02-1.554614347D-05
 9.513887120D-09-2.341473263D-12                 2.495863399D+04-1.779070154D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16150.258
-2.204028219D+05-1.072926248D+03 1.378367377D+01-3.093322915D-04 6.777528950D-08
-7.727301820D-12 3.566690220D-16                 2.431020015D+04-4.342161815D+01
C2CL4              Hf:  Manion,2002. Gurvich,1991 pt1 p115 pt2 p88.
 2 g 5/02 C   2.00CL  4.00     0.00     0.00     0.00 0  165.8322000      -24200.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19605.643
 3.746258300D+04-8.481775630D+02 1.009156110D+01 1.845463613D-02-2.390899444D-05
 1.514828257D-08-3.841119320D-12 0.000000000D+00-1.598288471D+03-2.368080605D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19605.643
-3.001315659D+05-1.132407598D+03 1.683072470D+01-3.288792490D-04 7.220907030D-08
-8.245332690D-12 3.810112780D-16 0.000000000D+00-2.292799594D+03-5.980161160D+01
C2CL6              Hf:Manion,2002. Gurvich,1991 pt1 p117 pt2 p90.
 2 g 5/02 C   2.00CL  6.00     0.00     0.00     0.00 0  236.7376000     -148200.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27129.390
 1.593451813D+05-2.606697136D+03 2.028011847D+01 1.769364822D-02-3.133105185D-05
 2.389395238D-08-6.893038300D-12 0.000000000D+00-9.038007640D+03-7.953073760D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27129.390
-5.577386320D+05-4.976491240D+02 2.237041989D+01-1.477759098D-04 3.257546580D-08
-3.727099210D-12 1.723801704D-16 0.000000000D+00-2.335223305D+04-8.381732120D+01
C2F                Gurvich,1991 pt1 p81 pt2 p59.
 2 tpis91 C   2.00F   1.00     0.00     0.00     0.00 0   43.0198032      353847.482
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10367.036
 1.249797213D+04-3.483876750D+02 5.755084350D+00 8.528685380D-04 2.353546435D-06
-2.804737097D-09 9.083575640D-13                 4.281525310D+04-6.437200960D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10367.036
 2.898776676D+05-2.016644658D+03 8.875045710D+00-5.166841130D-04 1.092094306D-07
-1.212216787D-11 5.482287680D-16                 5.241287920D+04-2.773089580D+01
C2FCL              Gurvich,1991 pt1 p141 pt2 p113.
 2 tpis91 C   2.00F   1.00CL  1.00     0.00     0.00 0   78.4728032      33766.399
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13876.507
 2.697675344D+04-7.414403180D+02 9.629604300D+00-3.865544930D-04 3.003347997D-06
-2.710191661D-09 7.737586890D-13                 5.500620390D+03-2.515774889D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13876.507
 3.471454890D+05-2.348461100D+03 1.206875617D+01-5.804698230D-04 1.212734340D-07
-1.334214186D-11 5.992556610D-16                 1.502061224D+04-4.252445687D+01
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Appendix D (*continued*)

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C2FCL3            Gurvich,1991 pt1 p145 pt2 p119.
 2 tpis91 C   2.00F   1.00CL  3.00    0.00    0.00 0  149.3788032    -166000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18731.914
 1.237282217D+04-4.703961840D+02 7.581621790D+00 2.305727066D-02-2.792144322D-05
 1.679699826D-08-4.077572440D-12                -2.031333976D+04-9.274637513D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18731.914
-2.829505545D+05-1.473853145D+03 1.707879074D+01-4.265213390D-04 9.357199850D-08
-1.067932796D-11 4.933261610D-16                -1.738433314D+04-6.197054796D+01
C2F2              Gurvich,1991 pt1 p82 pt2 p60.
 2 tpis91 C   2.00F   2.00    0.00    0.00    0.00 0   62.0182064    -144665.688
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13266.419
 1.776313572D+04-6.113280940D+02 8.663606800D+00 9.156381210D-04 2.363808425D-06
-2.753750054D-09 8.713935970D-13                -1.649611017D+04-2.165150307D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13266.419
 4.193890940D+05-2.715359989D+03 1.230403413D+01-6.649305540D-04 1.385254301D-07
-1.520813764D-11 6.819821030D-16                -4.179221940D+03-4.670386230D+01
C2F2CL2           Gurvich,1991 pt1 p143 pt2 p115. Eql mixture of isomers.
 2 tpis91 C   2.00F   2.00CL  2.00    0.00    0.00 0  132.9242064    -337837.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17936.029
-1.150433214D+05 2.032113595D+03-1.119750271D+01 8.342451400D-02-1.163698616D-04
 7.833092890D-08-2.070004069D-11                -5.208256810D+04 8.888322147D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17936.029
-8.702565660D+05 7.264724480D+02 1.530689121D+01 3.045597224D-04-7.045468040D-08
 8.285924340D-12-3.898581070D-16                -5.208888710D+04-4.998300753D+01
C2F3              Gurvich,1991 pt1 p83 pt2 p61.
 2 tpis91 C   2.00F   3.00    0.00    0.00    0.00 0   81.0166096    -228181.093
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14163.567
-2.614775016D+04 2.101767714D+02 2.328625080D+00 2.368943293D-02-2.416431591D-05
 1.224916093D-08-2.488670434D-12                -3.028566585D+04 1.699608790D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14163.567
-1.242603837D+05-2.137292446D+03 1.455051371D+01-6.093891980D-04 1.331427672D-07
-1.515124358D-11 6.984112060D-16                -1.977146179D+04-5.421039870D+01
C2F3CL            Gurvich,1991 pt1 p142 pt2 p114.
 2 tpis91 C   2.00F   3.00CL  1.00    0.00    0.00 0  116.4696096    -515200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17128.149
-8.122270310D+03-1.574007092D+02 5.041810290D+00 2.621692321D-02-2.843001445D-05
 1.537643979D-08-3.360730670D-12                -6.354049950D+04 2.792301872D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17128.149
-2.162724659D+05-2.195103372D+03 1.759605428D+01-6.282617290D-04 1.374166610D-07
-1.565004037D-11 7.218309900D-16                -5.515109500D+04-6.921931824D+01
C2F4              Gurvich,1991 pt1 p84 pt2 p62.
 2 tpis91 C   2.00F   4.00    0.00    0.00    0.00 0  100.0150128    -659500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16330.554
-9.991530070D+03-1.291088427D+02 4.504229050D+00 2.592029640D-02-2.630308720D-05
 1.316489777D-08-2.625017169D-12                -8.090447080D+04 3.274241470D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16330.554
-1.629915758D+05-2.603903955D+03 1.788488423D+01-7.397038010D-04 1.614460340D-07
-1.835820392D-11 8.457641070D-16                -7.006371660D+04-7.454165860D+01
C2F6              Gurvich,1991 pt1 p86 pt2 p64.
 2 g12/99 C   2.00F   6.00    0.00    0.00    0.00 0  138.0118192   -1344000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20272.040
-3.795371700D+04 7.998276400D+02-4.671561810D+00 7.501450990D-02-9.812116100D-05
 6.319807590D-08-1.622597311D-11                -1.675211878D+05 5.053759200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20272.040
-1.011551484D+06-9.422140710D+02 2.202553906D+01-1.314518750D-04 1.866045300D-08
-3.467118610D-12 2.488311205D-16                -1.657434402D+05-9.302161150D+01
C2H               Ervin, 1990. Jacox,1998. Peric,1990. Kanamori,1988.
 2 g 6/01 C   2.00H   1.00    0.00    0.00    0.00 0   25.0293400     566200.482
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10448.682
 1.343669487D+04-5.067970720D+02 7.772107410D+00-6.512339820D-03 1.030117855D-05
-5.880147670D-09 1.226901861D-12                 6.892269990D+04-1.871881626D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10448.682
 3.922334570D+06-1.204751703D+04 1.756172920D+01-3.655442940D-03 6.987685430D-07
-6.825162010D-11 2.719262793D-15                 1.433266627D+05-9.561634380D+01
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C2HCL             Hf:Manion,2002. Gurvich,1991 pt1 p129 pt2 p99.
 2 g 5/02 C   2.00H   1.00CL  1.00     0.00     0.00 0   60.4820400      226400.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11787.625
 1.329785007D+05-2.174542126D+03 1.497980854D+01-1.290343389D-02 1.602596678D-05
-9.152049510D-09 2.021223607D-12 0.000000000D+00 3.604801320D+04-5.958237870D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11787.625
 1.152145326D+06-4.461193000D+03 1.281366744D+01-6.797346760D-04 1.151382756D-07
-1.046641954D-11 3.949860520D-16 0.000000000D+00 5.233947560D+04-5.320654570D+01
C2HCL3            Hf:Manion,2002. Gurvich,1991 pt1 p134 pt2 p105.
 2 g 5/02 C   2.00H   1.00CL  3.00     0.00     0.00 0  131.3874400      -17500.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16604.624
 3.959231250D+04-5.178753580D+02 5.155028770D+00 2.816922486D-02-3.624741720D-05
 2.392074270D-08-6.362401960D-12 0.000000000D+00-1.534346259D+03 1.209374516D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16604.624
 6.049254660D+05-4.236992320D+03 1.846273557D+01-8.137195060D-04 1.551211545D-07
-1.584630634D-11 6.700932490D-16 0.000000000D+00 1.848285551D+04-7.698368760D+01
C2HF              Gurvich,1991 pt1 p99 pt2 p73.
 2 tpis91 C   2.00H   1.00F   1.00     0.00     0.00 0   44.0277432      41692.304
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11445.908
 9.161169110D+04-1.537245636D+03 1.133665074D+01-4.624729310D-03 5.877985460D-06
-2.690992345D-09 3.524719530D-13                 1.085902820D+04-4.023994380D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11445.908
 1.234347179D+06-4.819581960D+03 1.302337752D+01-7.495435820D-04 1.285452942D-07
-1.184559365D-11 4.536784760D-16                 3.236811710D+04-5.640791820D+01
C2HFCL2           Gurvich,1991 pt1 p155 pt2 p133. Eql mixture of isomers.
 2 tpis91 C   2.00H   1.00F   1.00CL  2.00     0.00 0  114.9337432     -168648.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16259.290
 3.117399823D+04-1.369505457D+02 1.176399869D+00 4.080776600D-02-5.418137800D-05
 3.613600660D-08-9.625862350D-12                -2.115142871D+04 2.146433160D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16259.290
 4.071243520D+05-3.808204520D+03 1.821144050D+01-7.278966060D-04 1.381532849D-07
-1.405342513D-11 5.920009720D-16                -2.676849943D+03-7.567353567D+01
C2HF2CL           Gurvich,1991 pt1 p153 pt2 p129. 1,1 cis & trans in equil.
 2 tpis91 C   2.00H   1.00F   2.00CL  1.00     0.00 0   98.4791464     -333654.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15262.754
 1.704437675D+05-1.667236861D+03 4.788788500D+00 4.444830010D-02-7.322197770D-05
 5.629347550D-08-1.654638029D-11                -3.291809760D+04-5.788593640D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15262.754
 5.830374700D+05-3.810317410D+03 1.799003171D+01-5.888210860D-04 1.002861284D-07
-9.149788100D-12 3.459985160D-16                -2.205875409D+04-7.590948533D+01
C2HF3             Gurvich,1991 pt1 p105 pt2 p79.
 2 tpis91 C   2.00H   1.00F   3.00     0.00     0.00 0   82.0245496     -491000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14327.512
-1.410969036D+04 3.687624920D+02-1.144797568D+00 3.956306020D-02-4.602001360D-05
 2.785149385D-08-6.903760080D-12                -6.226410330D+04 3.289661690D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14327.512
 6.917413780D+05-5.260301640D+03 1.915276614D+01-1.072493938D-03 2.099276744D-07
-2.195126633D-11 9.472702400D-16                -3.247640210D+04-8.750456950D+01
C2H2,acetylene    Hf:TRC(10/93) w-3040. Gurvich,1991 pt1 p47 pt2 p39.
 2 g 1/91 C   2.00H   2.00     0.00     0.00     0.00 0   26.0372800      228200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10005.839
 1.598112089D+05-2.216644118D+03 1.265707813D+01-7.979651080D-03 8.054992750D-06
-2.433307673D-09-7.529233180D-14                 3.712619060D+04-5.244338900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10005.839
 1.713847410D+06-5.929106660D+03 1.236127943D+01 1.314186993D-04-1.362764431D-07
 2.712655786D-11-1.302066204D-15                 6.266578970D+04-5.818960590D+01
C2H2,vinylidene   Chen,1989. Osamura,1981.
 2 g 5/01 C   2.00H   2.00     0.00     0.00     0.00 0   26.0372800      414788.368
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10874.168
-1.466042239D+04 2.789475593D+02 1.276229776D+00 1.395015463D-02-1.475702649D-05
 9.476298110D-09-2.567602217D-12                 4.736110180D+04 1.658225704D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10874.168
 1.940838725D+06-6.892718150D+03 1.339582494D+01-9.368968670D-04 1.470804368D-07
-1.220040365D-11 4.122391660D-16                 9.107112930D+04-6.337502930D+01
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C2H2CL2           Gurvich,1991 pt1 p130 pt2 p101. 1,1 cis & trans in equil.
 2 tpis91 C   2.00H   2.00CL  2.00    0.00    0.00 0   96.9432800       3410.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14882.477
-1.203724514D+04 4.629031190D+02-1.318184584D+00 3.930449600D-02-4.851529020D-05
 3.178411460D-08-8.476938410D-12                -3.251806860D+03 3.489218118D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14882.477
 1.561121185D+06-7.358096350D+03 2.011869185D+01-1.310978834D-03 2.411885716D-07
-2.384166740D-11 9.785415750D-16                 4.122200900D+04-9.550252712D+01
C2H2FCL           Gurvich,1991 pt1 p150 pt2 p125. 1,1 cis & trans in equil.
 2 tpis91 C   2.00H   2.00F   1.00CL  1.00    0.00 0   80.4886832     -165082.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13469.313
 2.260154427D+05-2.557428772D+03 9.236241200D+00 2.879408894D-02-5.163975470D-05
 4.252191030D-08-1.311612713D-11                -8.180627840D+03-3.234787581D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13469.313
 1.527690968D+06-6.689712230D+03 1.950553830D+01-1.040920895D-03 1.780587502D-07
-1.633098515D-11 6.213465560D-16                 1.705266451D+04-9.194078301D+01
C2H2F2            Gurvich,1991 pt1 p101 pt2 p75. 1,1 cis & trans in equil.
 2 tpis91 C   2.00H   2.00F   2.00    0.00    0.00 0   64.0340864     -336400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12479.683
 5.702935810D+04-6.762860400D+02 4.117411710D+00 1.822618762D-02-6.861331540D-06
-3.295756740D-09 2.180965597D-12                -3.838650780D+04 1.487528685D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12479.683
-8.227192750D+05-2.915718833D+03 1.830163995D+01-1.039630129D-03 2.546725128D-07
-3.157578705D-11 1.551540960D-15                -3.110028589D+04-8.400834700D+01
CH2CO,ketene      Wagman,1982. Moore,1963.
 2 g 7/00 C   2.00H   2.00O   1.00    0.00    0.00 0   42.0366800      -47700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11797.746
 3.503274040D+04-4.001693250D+02 3.691806430D+00 1.589408702D-02-1.733190594D-05
 1.161219965D-08-3.313412960D-12                -5.014866400D+03 2.848266196D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11797.746
 2.015132200D+06-8.200240060D+03 1.759005013D+01-1.460345107D-03 2.684671350D-07
-2.651382523D-11 1.087131348D-15                 4.200517260D+04-8.836222940D+01
O(CH)2O           Glyoxal. Dorofeeva,2001. Hubner,1997. Zeleznik,2002.
 2 g 3/02 C   2.00H   2.00O   2.00    0.00    0.00 0   58.0360800     -212000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13682.443
-2.292459698D+05 3.724098050D+03-1.893769993D+01 7.511744140D-02-8.083855420D-05
 4.358233190D-08-9.364539330D-12 0.000000000D+00-4.454486010D+04 1.327028760D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13682.443
 2.678063593D+05-4.436617480D+03 1.781696797D+01-7.097173780D-04 1.272621878D-07
-1.237226678D-11 5.025057520D-16 0.000000000D+00-4.479608280D+03-8.156700640D+01
HO(CO)2OH         Oxalic Acid, HO-CO-CO-OH. Dorofeeva,2001.
 2 srd 01 C   2.00H   2.00O   4.00    0.00    0.00 0   90.0348800     -731800.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17321.662
 3.072513274D+04-3.916174690D+02 3.178388640D+00 3.741289750D-02-4.009753960D-05
 2.288662646D-08-5.386771550D-12 0.000000000D+00-8.797942550D+04 9.751091370D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17321.662
 1.805560696D+06-9.240333150D+03 2.625742604D+01-1.418458557D-03 2.526840574D-07
-2.521005198D-11 1.040036111D-15 0.000000000D+00-3.754286460D+04-1.326879788D+02
C2H3,vinyl        Radical. Ervin,1990.
 2 g 7/01 C   2.00H   3.00    0.00    0.00    0.00 0   27.0452200      299686.817
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10521.791
-3.347896870D+04 1.064104103D+03-6.403857060D+00 3.934515480D-02-4.760046090D-05
 3.170071350D-08-8.633406430D-12                 3.039122649D+04 5.809226180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10521.791
 2.718080093D+06-1.030956829D+04 1.836579807D+01-1.580131153D-03 2.680594939D-07
-2.439003999D-11 9.209096390D-16                 9.765055590D+04-9.760086860D+01
CH2Br-COOH        Bromoacetic Acid. Dorofeeva,2001.
 2 srd 01 C   2.00H   3.00BR  1.00O   2.00    0.00 0  138.9480200     -383500.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16862.437
-7.832484790D+04 1.648865353D+03-9.349533630D+00 6.879635440D-02-8.374880770D-05
 5.406038420D-08-1.423159923D-11 0.000000000D+00-5.541187620D+04 8.165423200D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16862.437
 2.486349850D+06-1.140256346D+04 2.756020307D+01-1.843187010D-03 3.265392740D-07
-3.122663159D-11 1.223452495D-15 0.000000000D+00 1.837013127D+04-1.420040888D+02
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C2H3CL            Hf:Manion,2002. Gurvich,1991 pt1 p129 pt2 p100.
 2 g 5/02 C   2.00H   3.00CL  1.00    0.00    0.00 0   62.4979200      22000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11819.647
-1.688895457D+04 8.545104550D+02-6.514967550D+00 4.944681930D-02-6.117756670D-05
 4.067293850D-08-1.101392611D-11 0.000000000D+00-2.069321321D+03 5.928434500D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11819.647
 2.456176938D+06-1.047452327D+04 2.178736181D+01-1.816891849D-03 3.296369950D-07
-3.214395690D-11 1.302254061D-15 0.000000000D+00 6.346228700D+04-1.149890578D+02
CH2CL-COOH        Chloroacetic Acid. Dorofeeva,2001.
 2 srd 01 C   2.00H   3.00CL  1.000   2.00    0.00 0   94.4967200    -427600.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16513.941
-1.122506518D+05 2.168288658D+03-1.227791286D+01 7.514388250D-02-9.083158770D-05
 5.812364190D-08-1.518247503D-11 0.000000000D+00-6.314314550D+04 9.694389590D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16513.941
 2.472883176D+06-1.152275963D+04 2.766275606D+01-1.886430963D-03 3.361776050D-07
-3.231272250D-11 1.273275883D-15 0.000000000D+00 1.370387108D+04-1.443191401D+02
C2H3F             Gurvich,1991 pt1 p100 pt2 p74.
 2 tpis91 C   2.00H   3.00F   1.00    0.00    0.00 0   46.0436232    -140100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11335.928
-4.579134960D+04 1.411541724D+03-1.021500877D+01 5.775816570D-02-7.080677490D-05
 4.640850760D-08-1.240455865D-11                -2.402788827D+04 7.860828390D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11335.928
 2.478832340D+06-1.075932307D+04 2.194796688D+01-1.869114110D-03 3.395280670D-07
-3.315382930D-11 1.345081799D-15                 4.563455550D+04-1.180410277D+02
CH3CN             Acetonitrile. TRC(6/93) w9270. Koga,1984. Pavone,1990.
 2 g 9/00 C   2.00H   3.00N   1.00    0.00    0.00 0   41.0519200      66430.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12093.688
-9.965988380D+04 1.739278534D+03-7.898420820D+00 4.294894320D-02-4.499973880D-05
 2.717105086D-08-7.026117590D-12                -1.461161333D+03 6.852508274D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12093.688
 2.923231393D+06-1.233792258D+04 2.324477222D+01-2.411565845D-03 4.622157170D-07
-4.740601240D-11 2.010639467D-15                 8.058565550D+04-1.292249102D+02
CH3CO,acetyl      Radical. Hf:Niiranen,1992. Nimlos,1989.
 2 g 6/96 C   2.00H   3.00O   1.00    0.00    0.00 0   43.0446200     -10000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13036.467
-7.193894130D+04 1.464465167D+03-6.632276130D+00 4.108468380D-02-4.226256640D-05
 2.485766819D-08-6.292558480D-12                -9.309370810D+03 6.422897620D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13036.467
 2.485388150D+06-1.120714204D+04 2.277525438D+01-2.314260550D-03 4.536189170D-07
-4.742635550D-11 2.044663903D-15                 6.380088410D+04-1.215350925D+02
C2H4              TRC(4/88) w2600. Chao,1975. Knippers,1985.
 2 g 1/00 C   2.00H   4.00    0.00    0.00    0.00 0   28.0531600      52500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10518.689
-1.163605836D+05 2.554851510D+03-1.609746428D+01 6.625779320D-02-7.885081860D-05
 5.125224820D-08-1.370340031D-11                -6.176191070D+03 1.093338343D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10518.689
 3.408763670D+06-1.374847903D+04 2.365898074D+01-2.423804419D-03 4.431395660D-07
-4.352683390D-11 1.775410633D-15                 8.820429380D+04-1.371278108D+02
C2H4O,ethylen-o   Ethylene Oxide. Shimanouchi,1972. Chase,1998 9/65.
 2 g 8/88 C   2.00H   4.00O   1.00    0.00    0.00 0   44.0525600     -52634.720
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10830.615
-1.728233345D+05 3.816678800D+03-2.629851977D+01 1.014103162D-01-1.240578373D-04
 8.034040350D-08-2.120942544D-11                -2.437519333D+04 1.654885056D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10830.615
 3.151809957D+06-1.423646316D+04 2.708080476D+01-2.606238456D-03 4.853891930D-07
-4.852144760D-11 2.011778721D-15                 7.662561440D+04-1.563952401D+02
CH3CHO,ethanal    Hf:TRC (6/78) w5300. Chao,1986.
 2 g 8/88 C   2.00H   4.00O   1.00    0.00    0.00 0   44.0525600     -166190.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12896.716
-1.373904369D+05 2.559937679D+03-1.340470172D+01 5.922128620D-02-6.240006050D-05
 3.703324410D-08-9.342697410D-12                -3.318731310D+04 1.007417652D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12896.716
 3.321176590D+06-1.449719957D+04 2.708421279D+01-2.879320054D-03 5.556309920D-07
-5.732674880D-11 2.443965239D-15                 6.507755640D+04-1.536236027D+02
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Appendix D (*continued*)

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CH3COOH          Acetic Acid. Chao,1978.
 2 g 6/00 C   2.00H   4.00O   2.00    0.00    0.00 0   60.0519600    -432249.040
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13597.391
-3.219191980D+04 1.196329795D+03-8.705824020D+00 5.696257590D-02-5.757887160D-05
 3.352115220D-08-8.614438230D-12                -5.840112870D+04 7.282413920D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13597.391
 2.103514223D+06-1.467822192D+04 3.382802830D+01-5.694858680D-03 1.343221353D-06
-1.606041158D-10 7.652794250D-15                2.924228407D+04-1.935278850D+02
OHCH2COOH        Glycolic Acid. Dorofeeva,2001.
 2 srd 01 C   2.00H   4.00O   3.00    0.00    0.00 0   76.0513600    -583000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17007.039
-3.138978580D+05 5.693068770D+03-3.685160290D+01 1.563502811D-01-2.039487993D-04
 1.340232412D-07-3.509130260D-11 0.000000000D+00-9.801640090D+04 2.269492355D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17007.039
 1.946628253D+06-9.804020200D+03 2.844111243D+01-7.876404750D-04 6.416275950D-08
 1.069321262D-12-3.237178280D-16 0.000000000D+00-1.694650470D+04-1.474109363D+02
C2H5             Chen,1990.
 2 g 7/00 C   2.00H   5.00    0.00    0.00    0.00 0   29.0611000     118658.240
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12185.226
-1.411312551D+05 2.714285088D+03-1.534977725D+01 6.451672580D-02-7.259143960D-05
 4.599116010D-08-1.218367535D-11                5.981418840D+02 1.090966520D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12185.226
 4.169220400D+06-1.662982142D+04 2.795442134D+01-3.051715761D-03 5.685160040D-07
-5.682863600D-11 2.355648561D-15                1.137010087D+05-1.639357995D+02
C2H5Br           Bromoethane. TRC(6/79) tuvw7650.
 2 n 6/79 C   2.00H   5.00BR  1.00    0.00    0.00 0  108.9651000     -63600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13569.000
-1.374172662D+05 2.861429418D+03-1.824108956D+01 8.566230600D-02-1.047174473D-04
 6.906074570D-08-1.862276022D-11               -2.198480205D+04 1.258435579D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13569.000
 2.378649403D+06-1.267033647D+04 2.777558646D+01-2.010898783D-03 4.436083410D-07
-5.348198090D-11 2.639835850D-15                6.414062050D+04-1.528277085D+02
C2H6             Ethane. Pamidimukkala,1982.
 2 g 7/00 C   2.00H   6.00    0.00    0.00    0.00 0   30.0690400     -83851.544
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11891.594
-1.862044161D+05 3.406191860D+03-1.951705092D+01 7.565835590D-02-8.204173220D-05
 5.061135800D-08-1.319281992D-11               -2.702932890D+04 1.298140496D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11891.594
 5.025782130D+06-2.033022397D+04 3.322552930D+01-3.836703410D-03 7.238405860D-07
-7.319182500D-11 3.065468699D-15                1.115963950D+05-2.039410584D+02
CH3N2CH3         Azomethane. Pamidumukkala,1982.
 2 g 8/88 C   2.00H   6.00N   2.00    0.00    0.00 0   58.0824400     148699.360
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16524.999
-3.738492320D+05 5.880453130D+03-2.986398524D+01 1.087380861D-01-1.167950177D-04
 6.916894890D-08-1.719950055D-11               -1.189984084D+04 1.948246321D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16524.999
 4.993357090D+06-2.160996161D+04 3.964449920D+01-4.196450110D-03 8.023361980D-07
-8.212260020D-11 3.477237440D-15                1.449962610D+05-2.372109745D+02
C2H5OH           Hf:TRC(6/87) w5030. Chao,1986.
 2 g 8/88 C   2.00H   6.00O   1.00    0.00    0.00 0   46.0684400    -234950.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14541.926
-2.342791392D+05 4.479180550D+03-2.744817302D+01 1.088679162D-01-1.305309334D-04
 8.437346400D-08-2.234559017D-11               -5.022229000D+04 1.764829211D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14541.926
 4.694817650D+06-1.929798213D+04 3.447584040D+01-3.236165980D-03 5.784947720D-07
-5.564600270D-11 2.226226400D-15                8.601622710D+04-2.034801732D+02
CH3OCH3          Dimethyl ether. Hf:TRC(6/91) w6040. Chao,1986.
 2 g 7/00 C   2.00H   6.00O   1.00    0.00    0.00 0   46.0684400    -184110.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14354.379
-2.693103242D+05 4.300709710D+03-2.152788028D+01 8.131833390D-02-8.295671320D-05
 4.801911510D-08-1.188699808D-11               -4.410237090D+04 1.467666934D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14354.379
 4.933577190D+06-2.083094065D+04 3.629050610D+01-4.108351640D-03 7.903220310D-07
-8.131435630D-11 3.458166110D-15                1.013301012D+05-2.185447466D+02
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CH3O2CH3          Dimethyl peroxide, CH3-O-O-CH3. Dorofeeva,2001.
 2 srd 01 C   2.00H   6.000   2.00    0.00    0.00 0   62.0678400    -125500.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17153.436
-2.285784757D+05 3.820142570D+03-1.976647823D+01 8.840743860D-02-9.641284560D-05
 5.907200830D-08-1.526491225D-11 0.000000000D+00-3.492016960D+04 1.386769151D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17153.436
 5.316368470D+06-2.221267874D+04 4.034335090D+01-4.612748090D-03 8.792987200D-07
-9.068221190D-11 3.865664890D-15 0.000000000D+00 1.161596028D+05-2.395296055D+02
CCN               Hf:Gurvich,1991 pt1 p222. Jacox,1998 p173.
 2 g 7/00 C   2.00N   1.00    0.00    0.00    0.00 0   38.0281000     804596.472
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11038.524
-1.696281385D+04 9.837891630D+01 3.812662940D+00 5.346894230D-03-2.473598508D-06
-3.730564220D-10 4.481756860D-13                 9.480072570D+04 5.553165572D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11038.524
 7.948674890D+04-1.344786906D+03 8.309986460D+00-2.220105361D-04 1.753683113D-08
 2.545998719D-12-2.645649117D-16                 1.023187495D+05-2.259793940D+01
CNC               CNC radical. Gurvich,1991 pt1 p221 pt2 p209.
 2 tpis91 C   2.00N   1.00    0.00    0.00    0.00 0   38.0281000     684914.559
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11356.611
-7.075192710D+04 1.007523898D+03-1.576789967D+00 2.052532634D-02-2.278935009D-05
 1.283362343D-08-2.933174091D-12                 7.613324850D+04 3.487094132D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11356.611
-9.031313560D+04-8.313236500D+02 8.114735950D+00-2.447691991D-04 5.397508770D-08
-6.183984860D-12 2.865172411D-16                 8.451833600D+04-2.102937255D+01
OCCN              Cyanooxomethyl radical. Dorofeeva,2001.
 2 srd 01 C   2.00N   1.00O   1.00    0.00    0.00 0   54.0275400     210000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13594.351
 2.428801276D+04-5.525864620D+02 8.587838170D+00-3.379387770D-03 1.119841826D-05
-1.008408077D-08 3.086448824D-12 0.000000000D+00 2.599620072D+04-1.659592359D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13594.351
 9.359131680D+05-4.441082290D+03 1.368959297D+01-1.647530917D-03 3.819873440D-07
-3.945161000D-11 1.509598839D-15 0.000000000D+00 4.951222780D+04-5.417089680D+01
C2N2              Gurvich,1979 pt1 p195 pt2 p220.
 2 tpis79 C   2.00N   2.00    0.00    0.00    0.00 0   52.0348000     309100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12715.153
 1.082404484D+05-1.928137871D+03 1.553891898D+01-1.821159329D-02 2.778840840D-05
-1.899434373D-08 4.949677720D-12                 4.449097590D+04-6.090964741D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12715.153
 7.934423720D+05-3.997376270D+03 1.314497430D+01-8.747782000D-04 2.059156733D-07
-2.200469389D-11 9.974485770D-16                 5.863632300D+04-5.473201251D+01
C2O               Hf:Gurvich,1991 pt1 p31. Jacox,1998.
 2 g 8/00 C   2.00O   1.00    0.00    0.00    0.00 0   40.0208000     291038.666
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10485.718
-3.959929420D+03-1.117516348D+02 4.593960060D+00 3.710602020D-03-7.014760180D-07
-1.371129839D-09 7.123854000D-13                 3.410109740D+04 4.622805600D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10485.718
-6.348056590D+05 1.184133091D+03 4.879173340D+00 1.757538773D-03-3.957552270D-07
 3.989179940D-11-1.546043135D-15                 2.489803938D+04 9.809040590D-01
C2S2              TRC(6/01) p8150, tuvw-8150.
 2 n 6/01 C   2.00S   2.00    0.00    0.00    0.00 0   88.1514000     376660.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13760.000
 4.192544750D+04-9.776562320D+02 1.085003376D+01-4.423407890D-03 1.067980519D-05
-8.781148100D-09 2.538862361D-12                 4.789590500D+04-3.097681854D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13760.000
 8.629908790D+05-4.325413740D+03 1.460010162D+01-1.460638433D-03 2.778253364D-07
-2.755649209D-11 1.105350739D-15                 6.839748750D+04-5.986379853D+01
C3                Gurvich,1979 pt2 p23.
 3 tpis79 C   3.00    0.00    0.00    0.00    0.00 0   36.0321000     839948.646
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12109.146
-4.354614480D+04 6.660183220D+02 1.451033157D+00 7.434513120D-03-3.810152990D-06
-2.336961396D-11 4.407054530D-13                 9.635170200D+04 2.025173297D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12109.146
 4.508098930D+06-1.461033761D+04 2.281974644D+01-8.544340610D-03 2.146069341D-06
-2.103867761D-10 6.351589060D-15                 1.911976065D+05-1.271869723D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12109.146
 1.539589859D+08-2.089057498D+05 7.681111210D+01-8.939056190D-03 5.594033240D-07
-1.743774353D-11 2.181541208D-16                 1.650801763D+06-6.081693320D+02
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C3H3,1-propynl    TRC(4/98) tuvw3140.
 2 n 4/98 C   3.00H   3.00    0.00    0.00    0.00 0   39.0559200     450000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12400.000
-6.505859350D+04 1.350858921D+03-5.825433930D+00 3.756610480D-02-3.734903340D-05
 2.117676603D-08-5.139113250D-12                 4.656510530D+04 5.781477550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12400.000
 4.550654870D+06-1.640574172D+04 2.712605991D+01-4.474600380D-03 1.037712415D-06
-1.250211369D-10 6.026582050D-15                 1.534087662D+05-1.565931809D+02
C3H3,2-propynl    TRC(4/98) tuvw3140.
 2 n 4/98 C   3.00H   3.00    0.00    0.00    0.00 0   39.0559200     331800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.000
 6.188578320D+04-8.909578670D+02 6.347558820D+00 1.633173115D-02-1.949975695D-05
 1.417349778D-08-4.199866320D-12                 4.271785830D+04-1.231400729D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.000
 2.989723833D+06-1.118954446D+04 2.222225052D+01-2.068106902D-03 4.121883640D-07
-4.438980590D-11 1.970824701D-15                 1.061878289D+05-1.186744583D+02
C3H4,allene       TRC(4/84) w2750. Shimanouchi,1972 p115. Butcher,1973a.
 2 g 2/00 C   3.00H   4.00    0.00    0.00    0.00 0   40.0638600     190920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12604.569
-1.645155745D+04 9.629457810D+02-7.532326680D+00 5.518219110D-02-6.733585120D-05
 4.532709050D-08-1.251837614D-11                 1.772494269D+04 6.151969760D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12604.569
 3.479355100D+06-1.430412453D+04 2.702534756D+01-2.557412369D-03 4.706646750D-07
-4.651688070D-11 1.908219044D-15                 1.072312354D+05-1.548846158D+02
C3H4,propyne      Hf:TRC(10/93) w3040. Trambarulo,1950. Shimanouchi,1972.
 2 g 1/00 C   3.00H   4.00    0.00    0.00    0.00 0   40.0638600     184900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13030.516
-3.563884400D+04 8.328139100D+02-4.073759440D+00 4.113929610D-02-4.470444950D-05
 2.847458197D-08-7.695298240D-12                 1.710206236D+04 4.516720950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13030.516
 3.710441420D+06-1.489145507D+04 2.732397127D+01-2.645264770D-03 4.858300350D-07
-4.794128480D-11 1.964338121D-15                 1.104898462D+05-1.567992462D+02
C3H4,cyclo-       Dorofeeva,1986.
 2 g 5/90 C   3.00H   4.00    0.00    0.00    0.00 0   40.0638600     277100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11373.663
-1.969520627D+04 1.505379338D+03-1.418206573D+01 7.642632960D-02-9.765583660D-05
 6.612003820D-08-1.811251145D-11                 2.625631782D+04 9.604631890D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11373.663
 3.168399580D+06-1.371044699D+04 2.664303646D+01-2.420408050D-03 4.427994130D-07
-4.351820200D-11 1.775948955D-15                 1.133683702D+05-1.522619086D+02
C3H5,allyl        Radical. Burcat,2001 p58.
 2 g 3/01 C   3.00H   5.00    0.00    0.00    0.00 0   41.0718000     163594.400
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12738.723
-4.315996140D+04 1.441600907D+03-1.197014426D+01 7.319796460D-02-9.066357850D-05
 6.077059450D-08-1.658826363D-11                 1.232157460D+04 8.563173240D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12738.723
 4.094570590D+06-1.676676186D+04 3.123006342D+01-2.885449982D-03 5.211343540D-07
-5.058284220D-11 2.039932554D-15                 1.185720481D+05-1.823070197D+02
C3H6,propylene    Hf:TRC(4/88) w2600. Chao,1975.
 2 g 2/00 C   3.00H   6.00    0.00    0.00    0.00 0   42.0797400      20000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13550.558
-1.912462174D+05 3.542074240D+03-2.114878626D+01 8.901484790D-02-1.001429154D-04
 6.267959390D-08-1.637870781D-11                -1.529961824D+04 1.407641382D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13550.558
 5.017620340D+06-2.086084035D+04 3.644156340D+01-3.881191170D-03 7.278677190D-07
-7.321204500D-11 3.052176369D-15                 1.261245355D+05-2.195715757D+02
C3H6,cyclo-       Dorofeeva,1986. Butcher,1973b.
 2 g 1/00 C   3.00H   6.00    0.00    0.00    0.00 0   42.0797400      53300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11409.981
-1.565787770D+05 4.111129870D+03-3.233447460D+01 1.306337881D-01-1.645563833D-04
 1.095708326D-07-2.956394783D-11                -1.245271686D+04 1.931559109D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11409.981
 4.785000670D+06-2.042118175D+04 3.631495780D+01-3.561319440D-03 6.476241240D-07
-6.328430100D-11 2.568705857D-15                 1.268274126D+05-2.223729099D+02
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C3H6O,propylox    TRC(6/84) w6150. Swalen,1957. Oetting,1964. Villarreal,1975.
 2 g 6/01 C   3.00H   6.000   1.00    0.00    0.00 0   58.0791400     -93720.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14405.453
-2.292808804D+05 4.495750540D+03-2.941117945D+01 1.213113827D-01-1.440060464D-04
 9.202051750D-08-2.416278343D-11                -3.317697210D+04 1.846878218D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14405.453
 4.789729990D+06-2.106895971D+04 3.954647730D+01-3.910929980D-03 7.325531510D-07
-7.357085970D-11 3.060618500D-15                 1.120344540D+05-2.372004192D+02
C3H6O,acetone     Chao,1986. Chao,1976.
 2 g 6/97 C   3.00H   6.000   1.00    0.00    0.00 0   58.0791400    -217149.600
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16193.193
-2.277802525D+05 4.215280010D+03-2.415785316D+01 9.907483320D-02-1.084940903D-04
 6.583355960D-08-1.676046146D-11                -4.726243940D+04 1.607926432D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16193.193
 5.001601920D+06-2.170155542D+04 3.964493990D+01-4.179945050D-03 7.962429530D-07
-8.122558050D-11 3.428780960D-15                 1.015145028D+05-2.368533477D+02
C3H6O,propanal    Hf:TRC(6/78) w5300. Chao,1986. Frankiss,1974.
 2 g 1/02 C   3.00H   6.000   1.00    0.00    0.00 0   58.0791400    -186000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17327.276
-2.655781702D+05 4.250640450D+03-2.109249262D+01 9.194256120D-02-1.004653044D-04
 6.133314820D-08-1.576298535D-11 0.000000000D+00-4.450371050D+04 1.456678605D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17327.276
 4.830933490D+06-2.075451152D+04 3.924855180D+01-4.095514000D-03 7.881692160D-07
-8.107684080D-11 3.437105430D-15 0.000000000D+00 9.944937880D+04-2.316690627D+02
C3H7,n-propyl     Radical. Tsang,1985.
 2 g 7/01 C   3.00H   7.00    0.00    0.00    0.00 0   43.0876800     100500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14860.058
-1.895337073D+05 3.949517260D+03-2.606216089D+01 1.121920441D-01-1.365292213D-04
 9.023662720D-08-2.441056990D-11                -7.227877440D+03 1.673705556D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14860.058
 5.646512940D+06-2.291087136D+04 3.987275180D+01-4.106232870D-03 7.562557770D-07
-7.478263020D-11 3.068983677D-15                 1.483006853D+05-2.403781190D+02
C3H7,i-propyl     Radical. Tsang,1985.
 2 g 9/85 C   3.00H   7.00    0.00    0.00    0.00 0   43.0876800      93300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14807.207
-2.952063445D+05 5.294432300D+03-3.105287013D+01 1.143871563D-01-1.291752393D-04
 8.057843760D-08-2.093908432D-11                -1.476815514D+04 1.988082360D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14807.207
 5.807002520D+06-2.411219997D+04 4.085288400D+01-4.517851330D-03 8.499427170D-07
-8.573514340D-11 3.583383960D-15                 1.546504050D+05-2.487098372D+02
C3H8              Hf:TRC(10/85) w1350. Chao,1973.
 2 g 2/00 C   3.00H   8.00    0.00    0.00    0.00 0   44.0956200    -104680.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14741.218
-2.433144337D+05 4.656270810D+03-2.939466091D+01 1.188952745D-01-1.376308269D-04
 8.814823910D-08-2.342987994D-11                -3.540335270D+04 1.841749277D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14741.218
 6.420731680D+06-2.659791134D+04 4.534356840D+01-5.020663920D-03 9.471216940D-07
-9.575405230D-11 4.009672880D-15                 1.455582459D+05-2.818374734D+02
C3H8O,1propanol   Hf:TRC(6/87) w5030.  Chao,1986.
 2 g 2/00 C   3.00H   8.000   1.00    0.00    0.00 0   60.0950200    -255200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17518.759
-2.616973337D+05 5.192376660D+03-3.296481160D+01 1.354568128D-01-1.593156164D-04
 1.019498160D-07-2.688552974D-11                -5.612854350D+04 2.085024431D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17518.759
 6.308672120D+06-2.642210376D+04 4.715112590D+01-4.642511930D-03 8.593465360D-07
-8.682091820D-11 3.642224010D-15                 1.255003155D+05-2.859463804D+02
C3H8O,2propanol   Hf:TRC(6/87) w5030.  Chao,1986.
 2 g 2/00 C   3.00H   8.000   1.00    0.00    0.00 0   60.0950200    -272700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17264.775
-3.386510240D+05 6.106048000D+03-3.791418040D+01 1.530494531D-01-1.864354461D-04
 1.213257738D-07-3.220433490D-11                -6.279959350D+04 2.334322610D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17264.775
 6.001074750D+06-2.505876830D+04 4.622096120D+01-4.272466310D-03 7.693678770D-07
-7.450584840D-11 2.998959935D-15                 1.148518732D+05-2.796132222D+02
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Appendix D (*continued*)

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CNCOCN              Oxopropanedinitrile, NC-CO-CN. Dorofeeva,2001.
 2 srd 01 C    3.00N    2.00O    1.00     0.00     0.00 0    80.0449800      247500.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17147.758
 1.131052075D+05-1.978834961D+03 1.626886206D+01-8.330803440D-03 1.884127045D-05
-1.530681289D-08 4.418125300D-12 0.000000000D+00 3.680261740D+04-5.963327280D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17147.758
 7.000522440D+05-5.086002010D+03 1.946753490D+01-1.302852727D-03 2.753600750D-07
-3.056290852D-11 1.382140838D-15 0.000000000D+00 5.539338880D+04-8.627550860D+01
C3OS                TRC(6/01) p8150, tuvw-8150.
 2 n 6/01 C    3.00O    1.00S    1.00     0.00     0.00 0    84.0965000      157330.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15720.000
 1.173396837D+05-2.154246274D+03 1.739096818D+01-1.606951508D-02 2.815913738D-05
-2.144517776D-08 6.117883960D-12                 2.690975728D+04-6.715503804D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15720.000
 4.650964090D+05-3.653583100D+03 1.589374854D+01-7.274431680D-04 1.507932631D-07
-1.250975180D-11 2.879103391D-16                 3.664221650D+04-6.509079314D+01
C3O2                Hf:Chase,1998 p690 6/68. Shimanouchi,1977 p1083.
 2 g 7/88 C    3.00O    2.00     0.00     0.00     0.00 0    68.0309000      -93638.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15084.983
 1.579873382D+05-2.529493506D+03 1.801761578D+01-1.786032042D-02 2.978671986D-05
-2.182900022D-08 6.013797220D-12                -1.121054014D+03-7.277721170D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15084.983
 6.968699890D+05-4.624733190D+03 1.663905725D+01-1.175486554D-03 2.478106444D-07
-2.745165984D-11 1.239566766D-15                 1.252580069D+04-7.275968780D+01
C3S2                TRC(6/01) p8150, tuvw-8150.
 2 n 6/01 C    3.00S    2.00     0.00     0.00     0.00 0   100.1621000      412500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15990.000
 9.328308590D+04-1.860679192D+03 1.613667767D+01-1.172634768D-02 2.228897169D-05
-1.808702234D-08 5.421828530D-12                 5.607264740D+04-6.032261795D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15990.000
 2.718212835D+05-2.941949284D+03 1.559075626D+01-8.093965740D-04 1.739434000D-07
-1.932034262D-11 8.570339980D-16                 6.274672550D+04-6.207028885D+01
C4                  Gurvich,1991 pt1 p18 pt2 p16.
 3 g tpis C    4.00     0.00     0.00     0.00     0.00 0    48.0428000     1033903.742
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13117.742
 3.903780500D+04-8.948280780D+02 1.050952925D+01-6.552894460D-03 1.243940464D-05
-8.645341370D-09 2.263638846D-12                 1.266425869D+05-3.077594475D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13117.742
 9.200685130D+05-1.530311800D+03 6.050069200D+00 5.252743670D-03-1.779154772D-06
 2.589873632D-10-1.385553481D-14                 1.334389611D+05-7.261148820D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13117.742
-2.864752103D+07 1.765535487D+04 6.166598280D+00 8.098789030D-04-6.653483810D-08
 2.504726897D-12-3.585724180D-17                -2.082319291D+04 4.331258920D+00
C4H2,butadiyne      1,3-Butadiyne. Dorofeeva,1991.
 2 g 7/01 C    4.00H    2.00     0.00     0.00     0.00 0    50.0586800      450000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14393.860
 2.467542569D+05-3.897855640D+03 2.366080456D+01-2.208077805D-02 2.781101140D-05
-1.577340010D-08 3.423165460D-12                 7.086907820D+04-1.109173560D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14393.860
 2.328179913D+06-8.925186090D+03 2.114326883D+01-1.368871276D-03 2.327503159D-07
-2.124517624D-11 8.053313020D-16                 1.057788416D+05-1.088313574D+02
C4H4,1,3-cyclo-     1,3-Cyclobutadiene. Dorofeeva,1986.
 2 g 8/00 C    4.00H    4.00     0.00     0.00     0.00 0    52.0745600      385000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12103.534
-2.778428049D+04 1.768176915D+03-1.757895171D+01 9.383512920D-02-1.195524281D-04
 7.978086190D-08-2.152751100D-11                 3.811627120D+04 1.128478124D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12103.534
 2.991498949D+06-1.416781502D+04 3.001978876D+01-2.579200423D-03 4.789990450D-07
-4.775329710D-11 1.974923662D-15                 1.274666920D+05-1.727532057D+02
C4H6,butadiene      1,3-butadiene. TRC(10/92) tuvw2820.
 2 n10/92 C    4.00H    6.00     0.00     0.00     0.00 0    54.0904400      110000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15130.000
-9.181130530D+04 3.312570530D+03-2.985828611D+01 1.479201147D-01-2.056618326D-04
 1.466496826D-07-4.145285730D-11                -2.077309444D+03 1.780687329D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15130.000
-2.361903188D+07 5.651323370D+04-3.275738320D+01 2.293070572D-02-2.297106441D-06
 4.292596210D-11 4.236766040D-15                -3.671358620D+05 3.013437302D+02
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Appendix D (*continued*)

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C4H6,1butyne      TRC(10/93) tuvw3040.
 2 n10/93 C   4.00H   6.00    0.00    0.00    0.00 0   54.0904400     165200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16020.000
-5.597039970D+04 1.433191711D+03-9.691210720D+00 7.150002390D-02-8.157967800D-05
 5.290364970D-08-1.435655372D-11                  1.184987013D+04 7.660225360D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16020.000
 6.364402700D+06-2.392087731D+04 4.073750410D+01-3.176726490D-03 1.199856984D-07
 3.201802510D-11-2.854392633D-15                  1.634335546D+05-2.460284791D+02
C4H6,2butyne      TRC(10/93) tuvw3040.
 2 n10/93 C   4.00H   6.00    0.00    0.00    0.00 0   54.0904400     145700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16640.000
-2.650756405D+05 4.490728690D+03-2.400723889D+01 9.819579550D-02-1.079717182D-04
 6.675555770D-08-1.740766886D-11                 -5.328363710D+03 1.595035268D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16640.000
 3.981304330D+06-1.873032899D+04 3.654561490D+01-2.369686378D-03 3.990211810D-07
-3.698707270D-11 1.442072006D-15                  1.261460214D+05-2.155866205D+02
C4H6,cyclo-       Cyclobutene. Dorofeeva,1986.
 2 g 8/00 C   4.00H   6.00    0.00    0.00    0.00 0   54.0904400     156700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12557.564
-2.046707734D+05 4.919470570D+03-3.753278160D+01 1.497293031D-01-1.860139375D-04
 1.219909019D-07-3.254073590D-11                 -3.915950540D+03 2.233282138D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12557.564
 4.517367820D+06-2.097311985D+04 4.008039170D+01-3.949793980D-03 7.448484990D-07
-7.529754170D-11 3.153253502D-15                  1.406469848D+05-2.434836999D+02
C4H8,1-butene     TRC(4/88) tuvw2600.
 2 n 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200      -540.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17120.000
-2.721492014D+05 5.100079250D+03-3.183786250D+01 1.317754442D-01-1.527359339D-04
 9.714761110D-08-2.560204470D-11                 -2.523096386D+04 2.006932108D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17120.000
 6.257948610D+06-2.660376305D+04 4.764920050D+01-4.383267110D-03 7.128838440D-07
-5.991020840D-11 2.051753504D-15                  1.569252657D+05-2.913869761D+02
C4H8,cis2-buten   Cis2-butene TRC(4/88) tuvw2600.
 2 n 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200      -7400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16800.000
-2.773870877D+05 5.382384040D+03-3.375188100D+01 1.322980623D-01-1.490975922D-04
 9.277722000D-08-2.408282948D-11                 -2.715884347D+04 2.114462085D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16800.000
 6.461018350D+06-2.775376432D+04 4.863532360D+01-4.862386350D-03 8.412626100D-07
-7.633890370D-11 2.861702826D-15                  1.630856187D+05-3.003105998D+02
C4H8,tr2-butene   TRC(4/88) tuvw-2600.
 2 n 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200     -11000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17510.000
-3.594644110D+05 5.930972080D+03-3.255825290D+01 1.254957780D-01-1.374705365D-04
 8.407341350D-08-2.163047345D-11                 -3.113296523D+04 2.070081219D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17510.000
 6.444758090D+06-2.750706151D+04 4.870329380D+01-4.952445460D-03 8.700135910D-07
-8.017471710D-11 3.052575093D-15                  1.612137505D+05-3.004419156D+02
C4H8,isobutene    TRC(4/88) tuvw2600.
 2 n 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200     -17100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17010.000
-2.327205032D+05 3.941994240D+03-2.224581184D+01 1.012790864D-01-1.073194065D-04
 6.454696910D-08-1.646330345D-11                 -2.233766063D+04 1.479597621D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17010.000
 6.484970990D+06-2.732504764D+04 4.836321080D+01-4.768004050D-03 8.233875840D-07
-7.449253000D-11 2.782303056D-15                  1.595941773D+05-2.982986237D+02
C4H8,cyclo-       Cyclobutane. Dorofeeva,1986.
 2 g 8/00 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200      28400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13534.163
-3.047655983D+05 6.519482730D+03-4.662987590D+01 1.743593052D-01-2.090964176D-04
 1.343528679D-07-3.542727400D-11                 -2.700031171D+04 2.738348195D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13534.163
 4.456213810D+06-2.301018492D+04 4.492448460D+01-3.080145176D-03 5.317165260D-07
-5.081079380D-11 2.048919092D-15                  1.355487603D+05-2.771801965D+02
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(CH3COOH)2          Acetic acid dimer. Chao,1978.
 2 g10/00 C   4.00H   8.000   4.00     0.00     0.00 0  120.1039200    -929015.360
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28053.169
-3.094720023D+05 5.983338600D+03-3.573002920D+01 1.662525587D-01-1.883866300D-04
 1.154939386D-07-2.935166753D-11                 -1.421493469D+05 2.295855147D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28053.169
 6.571327590D+06-3.036870720D+04 6.250376670D+01-5.732624710D-03 1.083461635D-06
-1.097963590D-10 4.609263380D-15                  6.347426600D+04-3.734555070D+02
C4H9,n-butyl        TRC(10/84) tuvw1940.
 2 n10/84 C   4.00H   9.00     0.00     0.00     0.00 0   57.1142600      66530.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19797.000
-2.239560407D+05 4.676554100D+03-2.985424449D+01 1.345493704D-01-1.600660350D-04
 1.045338096D-07-2.812951048D-11                 -1.525297704D+04 1.901651559D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19797.000
 7.198686940D+06-2.959241524D+04 5.242042810D+01-5.441572440D-03 9.917758370D-07
-9.464455870D-11 3.729487040D-15                  1.834566472D+05-3.214209170D+02
C4H9,i-butyl        2-methylpropyl. TRC(10/84) tuvw1940.
 2 n10/84 C   4.00H   9.00     0.00     0.00     0.00 0   57.1142600      57320.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18317.000
-2.399461281D+05 4.697444540D+03-3.087472560D+01 1.391655831D-01-1.670233968D-04
 1.092423088D-07-2.936209962D-11                 -1.638151036D+04 1.936662372D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18317.000
 6.752936060D+06-2.837423721D+04 5.140687610D+01-4.982399010D-03 8.801506630D-07
-8.125738690D-11 3.099140009D-15                  1.743448480D+05-3.149940745D+02
C4H9,s-butyl        1-methylpropyl radical. Tsang,1985.
 2 g 1/93 C   4.00H   9.00     0.00     0.00     0.00 0   57.1142600      71000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17537.649
-3.351062890D+05 6.312945950D+03-4.003025260D+01 1.563875047D-01-1.842331788D-04
 1.182727848D-07-3.131156589D-11                 -2.216045659D+04 2.481295714D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17537.649
 7.224744350D+06-3.035291099D+04 5.288551830D+01-5.652083550D-03 1.060032692D-06
-1.066129835D-10 4.443810960D-15                  1.883494279D+05-3.255719880D+02
C4H9,t-butyl        1,1dimethylethyl radical. Tsang,1985.
 2 g 1/93 C   4.00H   9.00     0.00     0.00     0.00 0   57.1142600      51700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17009.675
-4.723461950D+05 8.090198770D+03-4.683675340D+01 1.575300095D-01-1.686559436D-04
 9.981040130D-08-2.487608823D-11                 -3.319367410D+04 2.894838706D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17009.675
 7.151064950D+06-3.171224410D+04 5.442510320D+01-6.392331160D-03 1.241097612D-06
-1.287248300D-10 5.512618740D-15                  1.934506997D+05-3.399325290D+02
C4H10,n-butane      Hf:TRC(10/85) w1350. Chen,1975.
 2 g12/00 C   4.00H  10.00     0.00     0.00     0.00 0   58.1222000    -125790.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19228.685
-3.175872540D+05 6.176331820D+03-3.891562120D+01 1.584654284D-01-1.860050159D-04
 1.199676349D-07-3.201670550D-11                 -4.540363390D+04 2.379488665D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19228.685
 7.682322450D+06-3.256051510D+04 5.736732750D+01-6.197916810D-03 1.180186048D-06
-1.221893698D-10 5.250635250D-15                  1.774526560D+05-3.587918760D+02
C4H10,isobutane     TRC(10/85) w1350. Chen,1975.
 2 g 8/00 C   4.00H  10.00     0.00     0.00     0.00 0   58.1222000    -134990.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17936.500
-3.834469330D+05 7.000039640D+03-4.440026900D+01 1.746183447D-01-2.078195348D-04
 1.339792433D-07-3.551681630D-11                 -5.034018890D+04 2.658966497D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17936.500
 7.528018920D+06-3.202517060D+04 5.700161000D+01-6.060013090D-03 1.143975809D-06
-1.157061835D-10 4.846042910D-15                  1.728500802D+05-3.576176890D+02
C4N2                Hf:TRC(12/93) w8992. Khanna,1987. Brown,1989.
 2 g 6/01 C   4.00N   2.00     0.00     0.00     0.00 0   76.0562000     529200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17799.401
 1.587802866D+05-2.987184206D+03 2.348081602D+01-2.607502448D-02 4.042830030D-05
-2.804912444D-08 7.397652050D-12                  7.505299470D+04-1.017578250D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17799.401
 1.167686152D+06-6.198644180D+03 2.062070093D+01-1.518619449D-03 3.162361680D-07
-3.469922800D-11 1.555154128D-15                  9.667409390D+04-9.669734738D+01
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Appendix D (*continued*)

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C5                Gurvich,1991 pt1 p20 pt2 p18.
 3 g 8/00 C   5.00    0.00    0.00    0.00    0.00 0   60.0535000    1050924.332
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16191.831
-1.200801119D+04-5.553702910D+02 1.123828271D+01-4.347884520D-03 1.738987490D-05
-1.707945418D-08 5.574541910D-12                  1.262404627D+05-3.262308990D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16191.831
 2.172055356D+05-2.958510027D+03 1.561080967D+01-8.200361920D-04 1.776898025D-07
-2.009853583D-11 9.222677770D-16                  1.395208064D+05-6.433077180D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16191.831
 3.266863960D+06-2.666377675D+03 1.408383780D+01-6.620512140D-05 4.099789450D-09
-1.315689998D-13 1.711940703D-18                  1.405413771D+05-5.349354010D+01
C5H6,1,3cyclo-    1,3-Cyclopentadiene. Pedley,1986 p90. Dorofeeva,1986.
 2 g 5/90 C   5.00H   6.00    0.00    0.00    0.00 0   66.1011400     134300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13535.529
-1.886259728D+05 4.738220870D+03-3.888958010D+01 1.667438533D-01-2.141149581D-04
 1.438132328D-07-3.906478110D-11                 -5.667022010D+03 2.279898557D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13535.529
 4.428478190D+06-2.123547976D+04 4.309819010D+01-3.914783460D-03 7.311847010D-07
-7.327241190D-11 3.044403403D-15                  1.382542782D+05-2.605959678D+02
C5H8,cyclo-       Cyclopentene. Hf:TRC(10/92) w2840. Dorofeeva,1986.
 2 g 1/93 C   5.00H   8.00    0.00    0.00    0.00 0   68.1170200      33900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14857.179
-2.631114588D+05 5.987753490D+03-4.522244600D+01 1.804626339D-01-2.177216062D-04
 1.402022671D-07-3.699094300D-11                 -2.379504749D+04 2.660136401D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14857.179
 4.569848100D+06-2.406018294D+04 4.881006460D+01-3.413054980D-03 6.047001660D-07
-5.927495780D-11 2.447865390D-15                  1.413983093D+05-2.989533527D+02
C5H10,1-pentene   TRC(4/87) tuvw2500.
 2 n 4/87 C   5.00H  10.00    0.00    0.00    0.00 0   70.1329000     -21280.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21680.000
-5.340548130D+05 9.298917380D+03-5.667792450D+01 2.123100266D-01-2.571298290D-04
 1.666834304D-07-4.434080470D-11                 -4.790682180D+04 3.396036400D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21680.000
 3.744014970D+06-2.104485321D+04 4.736126990D+01-4.244201200D-04-3.898975050D-08
 1.367074243D-11-9.313194230D-16                  1.154091373D+05-2.786177449D+02
C5H10,cyclo-      Cyclopentane. Dorofeeva,1986.
 2 g 2/01 C   5.00H  10.00    0.00    0.00    0.00 0   70.1329000     -77100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15023.337
-4.141119710D+05 8.627592800D+03-6.202959980D+01 2.259910921D-01-2.682303330D-04
 1.706289935D-07-4.464050920D-11                 -4.931522140D+04 3.583916230D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15023.337
 7.501938730D+06-3.505864850D+04 6.322480750D+01-6.940356580D-03 1.337306593D-06
-1.377905033D-10 5.867357640D-15                  1.954925511D+05-4.026550900D+02
C5H11,pentyl      Radical. TRC(10/84) tuvw1941.
 2 n10/84 C   5.00H  11.00    0.00    0.00    0.00 0   71.1408400      45810.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24422.000
-4.653715920D+05 8.564220420D+03-5.295242890D+01 2.094288859D-01-2.561602906D-04
 1.692755961D-07-4.596788110D-11                 -3.641704270D+04 3.196862240D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24422.000
 5.697252900D+06-2.891706175D+04 5.811029680D+01-3.593995010D-03 4.419967630D-07
-1.509664551D-11-6.626964430D-16                  1.717009550D+05-3.522477120D+02
C5H11,t-pentyl    1,1-dimethylpropyl radical. Tsang,1985.
 2 g 1/93 C   5.00H  11.00    0.00    0.00    0.00 0   71.1408400      32600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19643.723
-5.152181980D+05 9.144327830D+03-5.602397890D+01 1.998204194D-01-2.239112591D-04
 1.375455547D-07-3.523833050D-11                 -4.036266610D+04 3.402811000D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19643.723
 8.602108260D+06-3.805205770D+04 6.649690370D+01-7.533860630D-03 1.451612787D-06
-1.495593207D-10 6.368022330D-15                  2.281858805D+05-4.169408550D+02
C5H12,n-pentane   TRC(10/85) tuvw1350.
 2 n10/85 C   5.00H  12.00    0.00    0.00    0.00 0   72.1487800    -146760.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24184.000
-2.768894625D+05 5.834283470D+03-3.617541480D+01 1.533339707D-01-1.528395882D-04
 8.191092000D-08-1.792327902D-11                 -4.665375250D+04 2.265544053D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24184.000
-2.530779286D+06-8.972593260D+03 4.536223260D+01-2.626989916D-03 3.135136419D-06
-5.318728940D-10 2.886896868D-14                  1.484616529D+04-2.516550384D+02
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C5H12,i-pentane   2-Methylbutane. TRC(10/85) tuvw1350.
 2 n10/85 C   5.00H  12.00     0.00     0.00     0.00 0   72.1487800     -153700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22008.000
-4.231903390D+05 6.497189100D+03-3.681126970D+01 1.532424729D-01-1.548790714D-04
 8.749897120D-08-2.070547710D-11                 -5.155416590D+04 2.309518218D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22008.000
 1.156888594D+07-4.556246870D+04 7.495443630D+01-7.845415580D-03 1.444393314D-06
-1.464370213D-10 6.230285000D-15                  2.544927135D+05-4.801985780D+02
CH3C(CH3)2CH3     2,2-Dimethylpropane (neopentane). TRC(10/85) tuvw1350.
 2 n10/85 C   5.00H  12.00     0.00     0.00     0.00 0   72.1487800     -167920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23179.000
-8.973222270D+06 1.289225617D+05-7.199344830D+02 2.056862183D+00-2.953159699D-03
 2.158893146D-06-6.268318770D-10                 -6.394932020D+05 4.020806360D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23179.000
 1.684705520D+07-5.979430570D+04 8.685451480D+01-9.621917600D-03 1.653363091D-06
-1.674727926D-10 7.372119360D-15                  3.458496820D+05-5.760466970D+02
C6D5,phenyl       Radical-d5. Burcat,1985.
 2 g 1/01 C   6.00D   5.00     0.00     0.00     0.00 0   82.1347100      315740.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15919.077
 2.012837008D+05-1.979349332D+03 2.628267500D+00 5.951865260D-02-6.081280450D-05
 3.381391650D-08-8.125429080D-12                  4.697247490D+04 3.354700980D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15919.077
 1.411628125D+06-1.362569472D+04 4.028984940D+01-3.490989270D-03 7.379612130D-07
-8.192244050D-11 3.705330970D-15                  1.088073731D+05-2.293621057D+02
C6D6              Benzene-d6. Burcat,1985.
 2 g 1/01 C   6.00D   6.00     0.00     0.00     0.00 0   84.1488120       58157.378
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16324.686
 2.762911236D+05-2.865868902D+03 5.395070430D+00 5.939315170D-02-6.023631180D-05
 3.381398570D-08-8.306046370D-12                  2.047083778D+04-2.011790696D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16324.686
 1.758057871D+06-1.572121558D+04 4.468162490D+01-4.003361920D-03 8.445434400D-07
-9.360556980D-11 4.228475530D-15                  8.962045360D+04-2.615332268D+02
C6H2              Dorofeeva,1991.
 2 g 2/93 C   6.00H   2.00     0.00     0.00     0.00 0   74.0800800      670000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19607.714
 2.903722964D+05-4.929751500D+03 3.189323210D+01-3.119447315D-02 4.325763680D-05
-2.732517022D-08 6.674446110D-12                  1.011898682D+05-1.530593012D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19607.714
 2.592848577D+06-1.083361978D+04 2.847459495D+01-1.876727704D-03 3.412134280D-07
-3.337392890D-11 1.356853889D-15                  1.418517294D+05-1.494853494D+02
C6H5,phenyl       Radical.Hf:TRC(10/89) w4270. Jacox,1989. NASA ab initio.
 2 g11/00 C   6.00H   5.00     0.00     0.00     0.00 0   77.1039000      337200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14154.633
-1.211278245D+05 3.529045580D+03-3.116903422D+01 1.467550630D-01-1.831398296D-04
 1.192576957D-07-3.149265860D-11                  2.420972928D+04 1.868799946D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14154.633
 3.670279230D+06-1.894601209D+04 4.180581820D+01-3.503914150D-03 6.561821740D-07
-6.594714450D-11 2.748094212D-15                  1.476744628D+05-2.475301142D+02
C6H5O,phenoxy     Phenoxy radical. Burcat,1985.
 2 g 8/00 C   6.00H   5.00O    1.00     0.00     0.00 0   93.1033000      47700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16208.094
-1.292264217D+05 3.406740680D+03-2.911367361D+01 1.459180378D-01-1.780202758D-04
 1.138615885D-07-2.967142152D-11                 -1.055026758D+04 1.770682011D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16208.094
 3.678640340D+06-1.972980806D+04 4.541184410D+01-3.751064390D-03 7.114450780D-07
-7.233328850D-11 3.045637067D-15                  1.163595961D+05-2.681058539D+02
C6H6              TRC(10/86)w3200. Pliva,1982,1983,1984. Shimanouchi,1972.
 2 g 8/00 C   6.00H   6.00     0.00     0.00     0.00 0   78.1118400       82880.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14195.691
-1.677340902D+05 4.404500040D+03-3.717377910D+01 1.640509559D-01-2.020812374D-04
 1.307915264D-07-3.444284100D-11                 -1.035455401D+04 2.169853345D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14195.691
 4.538575720D+06-2.260502547D+04 4.694007300D+01-4.206676830D-03 7.907994330D-07
-7.968302100D-11 3.328212080D-15                  1.391464686D+05-2.868751333D+02
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Appendix D (*continued*)

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C6H5OH,phenol      Burcat,1985.
 2 g 8/00 C   6.00H   6.000   1.00    0.00    0.00 0   94.1112400      -96399.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17496.700
-1.209418144D+05 3.378292270D+03-2.991846148D+01 1.567802942D-01-1.970937198D-04
 1.291815064D-07-3.424351260D-11                -2.779387017D+04 1.799708977D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17496.700
 4.462081570D+06-2.165521026D+04 4.815015050D+01-3.568282430D-03 6.327175730D-07
-6.039905720D-11 2.399168678D-15                 1.113726204D+05-2.860454446D+02
C6H10,cyclo-       Cyclohexene. Dorofeeva,1986.
 2 g 1/93 C   6.00H  10.00    0.00    0.00    0.00 0   82.1436000      -4600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17270.784
-3.750282210D+05 7.643876750D+03-5.510434760D+01 2.166231405D-01-2.545452198D-04
 1.607607304D-07-4.185248410D-11                -3.661073010D+04 3.202409460D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17270.784
 7.510128980D+06-3.556858210D+04 6.703034940D+01-7.045351870D-03 1.358166400D-06
-1.400074492D-10 5.964551700D-15                 2.060274332D+05-4.238197660D+02
C6H12,1-hexene     TRC(4/87) tuvw2500.
 2 n 4/87 C   6.00H  12.00    0.00    0.00    0.00 0   84.1594800      -41950.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26240.000
-6.668831650D+05 1.176864939D+04-7.270998330D+01 2.709398396D-01-3.333246400D-04
 2.182347097D-07-5.859468820D-11                -6.215780540D+04 4.286825640D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26240.000
 7.332906960D+05-1.448848641D+04 4.671215490D+01 3.172978470D-03-5.242646520D-07
 4.280355820D-11-1.472353254D-15                 6.697740410D+04-2.623643854D+02
C6H12,cyclo-       Cyclohexane. Dorofeeva,1986.
 2 g 6/90 C   6.00H  12.00    0.00    0.00    0.00 0   84.1594800     -123300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17544.814
-5.679987040D+05 1.034238704D+04-6.800041250D+01 2.387797658D-01-2.511890049D-04
 1.425293184D-07-3.407833190D-11                -6.404635160D+04 3.934808210D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17544.814
 5.225149470D+06-3.364194580D+04 7.174607470D+01-6.698979120D-03 1.318443254D-06
-1.390794789D-10 6.060102240D-15                 1.732537609D+05-4.546814170D+02
C6H13,n-hexyl      TRC(10/83) tuvw1930.
 2 n10/83 C   6.00H  13.00    0.00    0.00    0.00 0   85.1674200      25100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28983.000
-1.427278220D+06 2.248828093D+04-1.297492240D+02 4.279797330D-01-5.556013180D-04
 3.791256940D-07-1.048462404D-10                -1.060261015D+05 7.497186760D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28983.000
 5.967938620D+06-3.299023160D+04 6.869073440D+01-4.225009060D-03 5.496523820D-07
-2.292851471D-11-5.086341890D-16                 1.906978683D+05-4.185362000D+02
C6H14,n-hexane     TRC(4/85) tuvw1440.
 2 g 6/01 C   6.00H  14.00    0.00    0.00    0.00 0   86.1753600     -166920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28702.000
-5.815926700D+05 1.079097724D+04-6.633947030D+01 2.523715155D-01-2.904344705D-04
 1.802201514D-07-4.617223680D-11                -7.271544570D+04 3.938283540D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28702.000
-3.106625684D+06-7.346087920D+03 4.694131760D+01 1.693963977D-03 2.068996667D-06
-4.212141680D-10 2.452345845D-14                 5.237503120D+02-2.549967718D+02
C7H7,benzyl        Radical. Brouwer,1988. Hippler,1990.
 2 g 7/01 C   7.00H   7.00    0.00    0.00    0.00 0   91.1304800      210500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18554.892
-1.836764826D+05 4.102465660D+03-3.202406100D+01 1.588249575D-01-1.894466924D-04
 1.203649671D-07-3.136589637D-11                 5.266333230D+03 1.938751720D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18554.892
 5.297322160D+06-2.599909398D+04 5.509750790D+01-4.977661470D-03 9.463152430D-07
-9.639008860D-11 4.064470420D-15                 1.738382912D+05-3.343829550D+02
C7H8               Hf:TRC(4/98) w3510. Hitchcock,1975. Rudolph,1967.
 2 g 1/93 C   7.00H   8.00    0.00    0.00    0.00 0   92.1384200      50170.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17940.345
-2.877962220D+05 6.133941520D+03-4.574706760D+01 1.936895724D-01-2.304305304D-04
 1.459301178D-07-3.790796100D-11                -2.308402499D+04 2.693915042D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17940.345
 6.184538350D+06-2.990284056D+04 5.982005970D+01-5.696983960D-03 1.080748416D-06
-1.098702235D-10 4.624740220D-15                 1.782047857D+05-3.698082250D+02
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C7H8O,cresol-mx   Eql. mixture of isomers. Kudchadker,1978.
 2 g12/00 C   7.00H   8.00O   1.00     0.00     0.00 0  108.1378200     -132298.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21838.344
-2.441417503D+05 5.080877840D+03-3.789048040D+01 1.864945070D-01-2.269511868D-04
 1.458989279D-07-3.822403350D-11                 -4.093657830D+04 2.281352234D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21838.344
 6.017373450D+06-2.849882774D+04 6.081543070D+01-4.996807110D-03 9.134279950D-07
-8.979444110D-11 3.667756970D-15                  1.472218400D+05-3.674850140D+02
C7H14,1-heptene   TRC(4/87) tuvw2500.
 2 n 4/87 C   7.00H  14.00     0.00     0.00     0.00 0   98.1860600      -62760.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          30790.000
-7.449402840D+05 1.332179893D+04-8.281694380D+01 3.108065994D-01-3.786779920D-04
 2.446841042D-07-6.488763870D-11                 -7.217885010D+04 4.856671490D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          30790.000
-1.927608174D+06-9.125024420D+03 4.748177970D+01 6.067660530D-03-8.684859080D-07
 5.813995260D-11-1.473979569D-15                  2.600914656D+04-2.562880707D+02
C7H15,n-heptyl    TRC(10/83) tuvw1930.
 2 n10/83 C   7.00H  15.00     0.00     0.00     0.00 0   99.1940000       4390.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33543.000
-1.671733521D+06 2.640010250D+04-1.526867707D+02 5.027121410D-01-6.521014030D-04
 4.443488110D-07-1.227815006D-10                 -1.273754623D+05 8.783933320D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33543.000
 5.444527570D+06-3.456829290D+04 7.638651950D+01-3.298972000D-03 2.343496957D-07
 2.467674021D-11-3.162012849D-15                  1.939079354D+05-4.641424660D+02
C7H16,n-heptane   TRC(10/85) tuv1460. TRC(10/84) ptuv1010.
 2 n10/85 C   7.00H  16.00     0.00     0.00     0.00 0  100.2019400     -187780.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33221.000
-6.127432890D+05 1.184085437D+04-7.487188600D+01 2.918466052D-01-3.416795490D-04
 2.159285269D-07-5.655852730D-11                 -8.013408940D+04 4.407213320D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33221.000
 9.135632470D+06-3.923319690D+04 7.889780850D+01-4.654251930D-03 2.071774142D-06
-3.442539300D-10 1.976834775D-14                  2.050708295D+05-4.851104020D+02
C7H16,2-methylh   2-methylhexane. TRC(10/85) tuvw1460.
 2 n10/85 C   7.00H  16.00     0.00     0.00     0.00 0  100.2019400     -194600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          30920.000
-7.104777770D+05 1.191251120D+04-7.345339440D+01 2.902952369D-01-3.462767680D-04
 2.260184498D-07-6.128813920D-11                 -8.202147700D+04 4.320042290D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          30920.000
 1.289912969D+06-1.784340963D+03 1.083537673D+01 5.270609240D-02-1.886832314D-05
 2.432255843D-09-1.135553789D-13                 -1.637529884D+04-2.981862410D+01
C8H8,styrene      Ethenylbenzene. TRC(4/89) tuvw4490.
 2 n 4/89 C   8.00H   8.00     0.00     0.00     0.00 0  104.1491200      148300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20940.000
-2.686930520D+05 6.167999470D+03-4.836054940D+01 2.182873229D-01-2.738561832D-04
 1.810084981D-07-4.867750270D-11                 -1.140639978D+04 2.817679014D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20940.000
-6.629183620D+06 1.514594166D+04 1.609822364D+00 3.383318600D-02-1.093737395D-05
 1.338825116D-09-6.032534920D-14                 -8.997324150D+04 4.311282790D+01
C8H10,ethylbenz   Ethylbenzene. TRC(10/86) tuvw3200.
 2 n10/86 C   8.00H  10.00     0.00     0.00     0.00 0  106.1650000      29920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22280.000
-4.694940000D+05 9.307168360D+03-6.521769470D+01 2.612080237D-01-3.181753480D-04
 2.051355473D-07-5.401817350D-11                 -4.073870210D+04 3.780904360D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22280.000
 5.551564100D+06-2.831380598D+04 6.061240720D+01 1.042112857D-03-1.327426719D-06
 2.166031743D-10-1.142545514D-14                  1.642241062D+05-3.691769820D+02
C8H16,1-octene    TRC(4/87) tuvw2500.
 2 n 4/87 C   8.00H  16.00     0.00     0.00     0.00 0  112.2126400      -83590.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          35350.000
-9.281905220D+05 1.640974476D+04-1.015939534D+02 3.748001410D-01-4.590829400D-04
 2.965335340D-07-7.840445210D-11                 -8.952426080D+04 5.907594270D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          35350.000
-4.409336070D+06-4.383678800D+03 4.939154260D+01 7.912339630D-03-7.888669510D-07
 9.970212350D-12 1.913144872D-15                 -1.122619342D+04-2.577650649D+02
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C8H17,n-octyl     TRC(10/83) tuvw1930.
 2 n10/83 C   8.00H  17.00     0.00     0.00     0.00 0  113.2205800     -16320.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          38103.000
-1.934340995D+06 3.054979830D+04-1.767903454D+02 5.801596650D-01-7.517414010D-04
 5.112469030D-07-1.410193662D-10                -1.498894706D+05 1.013724329D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          38103.000
 5.632173390D+06-3.821143670D+04 8.637927500D+01-3.608931580D-03 2.544260445D-07
 2.908638837D-11-3.679549740D-15                 2.103135470D+05-5.262422830D+02
C8H18,n-octane    TRC(4/85) tuvw1490.
 2 n 4/85 C   8.00H  18.00     0.00     0.00     0.00 0  114.2285200     -208750.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          37780.000
-6.986647150D+05 1.338501096D+04-8.415165920D+01 3.271936660D-01-3.777209590D-04
 2.339836988D-07-6.010892650D-11                -9.026223250D+04 4.939222140D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          37780.000
 6.365406950D+06-3.105364657D+04 6.969162340D+01 1.048059637D-02-4.129621950D-06
 5.543226320D-10-2.651436499D-14                 1.500968785D+05-4.169895650D+02
C8H18,isooctane   2,2,4-Trimethylpentane. TRC(4/85) tuvw1490.
 2 n 4/85 C   8.00H  18.00     0.00     0.00     0.00 0  114.2285200     -224010.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          32170.000
-1.688758565D+05 3.126903227D+03-2.123502828D+01 1.489151508D-01-1.151180135D-04
 4.473216170D-08-5.554882070D-12                -4.468060620D+04 1.417455793D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          32170.000
 1.352765032D+07-4.663370340D+04 7.795313180D+01 1.423729984D-02-5.073593910D-06
 7.248232970D-10-3.819190110D-14                 2.541178017D+05-4.933887190D+02
C9H19,n-nonyl     TRC (10/83) tuvw1930.
 2 n10/83 C   9.00H  19.00     0.00     0.00     0.00 0  127.2471600     -37030.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          42664.000
-2.194880612D+06 3.468565780D+04-2.009261419D+02 6.580503110D-01-8.525930010D-04
 5.794638960D-07-1.597637099D-10                -1.723194608D+05 1.149114017D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          42664.000
 5.277361740D+06-4.025701960D+04 9.457296720D+01-2.940301447D-03 6.978106990D-09
 6.805250240D-11-5.907095330D-15                 2.165320614D+05-5.754449500D+02
C10H8,naphthale   Naphthalene. Chen,1979.
 2 g 3/01 C  10.00H   8.00     0.00     0.00     0.00 0  128.1705200     150580.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20713.076
-2.602845316D+05 6.237409570D+03-5.226095040D+01 2.397692776D-01-2.912244803D-04
 1.854944401D-07-4.816619270D-11                -1.114700880D+04 2.972139517D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20713.076
 5.906172110D+06-3.163229240D+04 7.030342030D+01-6.018865540D-03 1.142052144D-06
-1.161605689D-10 4.892844020D-15                 1.962567046D+05-4.347848950D+02
C10H21,n-decyl    TRC(10/83) tuvw1930.
 2 n10/83 C  10.00H  21.00     0.00     0.00     0.00 0  141.2737400     -57740.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          47224.000
-2.446511152D+06 3.870081300D+04-2.244388176D+02 7.343624970D-01-9.513525600D-04
 6.462970330D-07-1.781502862D-10                -1.941633889D+05 1.280987834D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          47224.000
 4.967237760D+06-4.242468440D+04 1.028853417D+02-2.324848180D-03-2.284233900D-07
 1.056127364D-10-8.068065900D-15                 2.235429890D+05-6.255191160D+02
C12H9,o-bipheny   o-Biphenyl radical. Burcat,1985.
 2 g 8/00 C  12.00H   9.00     0.00     0.00     0.00 0  153.1998600     427730.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26589.347
-3.595840820D+05 7.661378560D+03-5.873290460D+01 2.697557882D-01-3.229756680D-04
 2.032907100D-07-5.231316720D-11                 1.458414642D+04 3.392687110D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26589.347
 6.736469420D+06-3.632194350D+04 8.210239600D+01-7.502342860D-03 1.456251733D-06
-1.507145019D-10 6.436470430D-15                 2.555524521D+05-5.042462970D+02
C12H10,biphenyl   Burcat,1985.
 2 g 8/00 C  12.00H  10.00     0.00     0.00     0.00 0  154.2078000     182130.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26783.523
-3.671034050D+05 8.128412590D+03-6.390994570D+01 2.901422744D-01-3.509590740D-04
 2.230989996D-07-5.788470290D-11                -1.679263066D+04 3.633464190D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26783.523
 7.480385360D+06-3.928087230D+04 8.661482220D+01-7.946398570D-03 1.531868544D-06
-1.576450171D-10 6.700602730D-15                 2.438050641D+05-5.381381490D+02
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Appendix D (*continued*)

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Ca                Hf:Cox,1989. Sugar,1985. Gordon,1999.
 3 g 8/97 CA  1.00     0.00     0.00     0.00     0.00 0   40.0780000      177800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.063892786D+04 4.384548330D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 7.547341240D+06-2.148642662D+04 2.530849567D+01-1.103773705D-02 2.293249636D-06
-1.209075383D-10-4.015333268D-15                 1.585862323D+05-1.609512955D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 2.291781634D+09-1.608862960D+06 4.312466360D+02-5.396508990D-02 3.531856210D-06
-1.164403850D-10 1.527134223D-15                 1.258651434D+07-3.692101610D+03
Ca+               Sugar,1985. Gordon,1999.
 3 g 1/98 CA  1.00E  -1.00     0.00     0.00     0.00 0   40.0774514      773827.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 9.232417790D+04 5.077674980D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 3.747070820D+06-1.174707738D+04 1.672546969D+01-8.334797710D-03 2.394593294D-06
-2.988243468D-10 1.356563002D-14                 1.664329088D+05-9.582821260D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 9.117128410D+08-6.220428460D+05 1.683741136D+02-2.140862670D-02 1.452947686D-06
-4.920790880D-11 6.575369235D-16                 4.959472060D+06-1.422600719D+03
CaBr              Gurvich,1996a pt1 p471 pt2 p367.
 2 tpis96 CA  1.00BR  1.00     0.00     0.00     0.00 0  119.9820000     -24868.681
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9856.119
 5.693832620D+02-1.257513537D+02 5.001508330D+00-1.039868753D-03 1.377594927D-06
-8.949013960D-10 2.395658928D-13                -3.728103980D+03 1.784864847D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9856.119
 2.783236402D+06-8.458203730D+03 1.431756560D+01-5.430781680D-03 1.522218659D-06
-1.831824807D-10 7.864288660D-15                 4.931270680D+04-6.537001100D+01
CaBr2             Gurvich,1996a pt1 p474 pt2 p369.
 2 tpis96 CA  1.00BR  2.00     0.00     0.00     0.00 0  199.8860000     -387197.300
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15603.200
 1.572504318D+03-2.238551236D+02 8.388457890D+00-1.944164774D-03 2.397926088D-06
-1.556572350D-09 4.124309580D-13                -4.772106610D+04-1.074965233D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15603.200
-2.219846426D+04-4.463155330D+00 7.503755110D+00-1.641654626D-06 3.879428060D-10
-4.683424260D-14 2.259325541D-18                -4.885436820D+04-5.590324250D+00
CaCL              Gurvich,1996a pt1 p464 pt2 p363.
 2 tpis96 CA  1.00CL  1.00     0.00     0.00     0.00 0   75.5310000     -103772.885
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9595.115
 6.395335260D+03-2.249042269D+02 5.283278390D+00-1.447983237D-03 1.643742771D-06
-9.430104280D-10 2.237516133D-13                -1.270169000D+04-1.391964289D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9595.115
 1.629182545D+06-4.766223020D+03 9.658929770D+00-2.523044131D-03 5.833542160D-07
-4.101726990D-11 8.813177640D-17                 1.662599241D+04-3.398731174D+01
CaCL+             Gurvich,1996a pt1 p466 pt2 p364.
 2 tpis96 CA  1.00CL  1.00E  -1.00     0.00     0.00 0   75.5304514      467190.513
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9361.113
 2.285284542D+03-2.002872721D+02 4.936990190D+00-3.860973030D-04 8.686661880D-08
 1.470205680D-10-7.689315870D-14                 5.588277950D+04-6.359815341D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9361.113
 1.770280396D+05-5.891372390D+02 5.103368800D+00-2.356761168D-04 5.483732870D-08
 2.137973112D-14-5.572887310D-16                 5.853417250D+04-2.191253644D+00
CaCL2             Gurvich,1996a pt1 p470 pt2 p366.
 2 tpis96 CA  1.00CL  2.00     0.00     0.00     0.00 0  110.9840000     -485243.477
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14857.023
 1.106802030D+04-4.249108250D+02 9.134711860D+00-3.497185310D-03 4.242184630D-06
-2.719673231D-09 7.138268630D-13                -5.850346760D+04-1.808678294D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14857.023
-3.595768780D+04-8.796495630D+00 7.507256910D+00-3.129465934D-06 7.322886480D-10
-8.776403220D-14 4.210486040D-18                -6.066779660D+04-8.553523451D+00
CaF               Gurvich,1996a pt1 p456 pt2 p359.
 2 tpis96 CA  1.00F   1.00     0.00     0.00     0.00 0   59.0764032     -276403.790
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9132.110
 3.184235400D+04-4.918235090D+02 5.701120890D+00-1.465138218D-03 9.092930810D-07
-1.367585222D-10-5.106323380D-14                -3.197694110D+04-5.996662260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9132.110
 5.195882670D+05-1.512321567D+03 5.869276250D+00-3.882524480D-04-2.484582298D-08
 3.749915960D-11-3.470976450D-15                -2.488814584D+04-8.614663700D+00
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CaF+              Gurvich,1996a pt1 p460 pt2 p360.
 2 tpis96 CA  1.00F   1.00E  -1.00    0.00    0.00 0   59.0758546     260664.608
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9003.108
 4.158340800D+04-5.627661660D+02 5.687522150D+00-1.264710572D-03 6.669086480D-07
-6.926752820D-11-3.978714620D-14                 3.305119500D+04-6.974485010D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9003.108
-1.398670845D+05 2.191526375D+02 4.214324340D+00 2.142798048D-04-5.778672600D-08
 9.985756310D-12-6.059621880D-16                 2.841605897D+04 2.740342729D+00
CaF2              Gurvich,1996a pt1 p462 pt2 p362.
 2 tpis96 CA  1.00F   2.00    0.00    0.00    0.00 0   78.0748064    -790828.409
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12811.591
 5.909352290D+04-1.019733042D+03 1.013165309D+01-5.503506440D-03 5.629319980D-06
-3.115401465D-09 7.205525940D-13                -9.192608190D+04-2.639505950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12811.591
-8.280409440D+04-3.115950071D+01 7.023577370D+00-9.521000020D-06 2.118160895D-09
-2.440713888D-13 1.135135468D-17                -9.729466770D+04-7.546243340D+00
CaH               Gurvich,1996a pt1 p447 pt2 p353.
 2 tpis96 CA  1.00H   1.00    0.00    0.00    0.00 0   41.0859400     229409.105
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8705.105
-4.513782230D+04 7.629429210D+02-1.280874223D+00 1.318774659D-02-1.481595334D-05
 8.536573220D-09-1.989958945D-12                 2.300378814D+04 3.053421525D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8705.105
-2.696952529D+06 8.607059750D+03-7.027454820D+00 7.467916310D-03-2.318610699D-06
 3.423072420D-10-1.892679792D-14                -2.773819107D+04 7.845822010D+01
CaI               Gurvich,1996a pt1 p474 pt2 p370.
 2 tpis96 CA  1.00I   1.00    0.00    0.00    0.00 0  166.9824700     12183.320
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10018.120
-8.261790180D+02-8.508975900D+01 4.864171690D+00-7.863169650D-04 1.100493506D-06
-7.348030610D-10 2.010892767D-13                 5.236753440D+02 3.585391680D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10018.120
 1.771071309D+06-5.683643730D+03 1.153857476D+01-4.194020200D-03 1.291359961D-06
-1.730043579D-10 8.380762350D-15                 3.583293200D+04-4.405917570D+01
CaI2              Gurvich,1996a pt1 p477 pt2 p372.
 2 tpis96 CA  1.00I   2.00    0.00    0.00    0.00 0  293.8869400    -259319.505
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16050.995
-1.097851401D+03-1.459821761D+02 8.089341840D+00-1.305332923D-03 1.624199331D-06
-1.061194001D-09 2.825551217D-13                -3.272692980D+04-6.981714940D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16050.995
-1.623727104D+04-2.859530722D+00 7.502432190D+00-1.071178707D-06 2.544559095D-10
-3.083631004D-14 1.491836724D-18                -3.346341170D+04-3.567305740D+00
CaO               Gurvich,1996a pt1 p443 pt2 p349.
 3 tpis96 CA  1.00O   1.00    0.00    0.00    0.00 0   56.0774000     38005.308
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8953.108
 3.889733070D+04-4.835677350D+02 5.077713250D+00 3.076235250D-04-1.159759897D-06
 8.493433340D-10-1.495333366D-13                 5.937643480D+03-3.955320730D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8953.108
-4.913106170D+07 1.495865950D+05-1.681654149D+02 9.381950260D-02-2.455529428D-05
 3.074980720D-09-1.485914237D-13                -9.461511720D+05 1.235694769D+03
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8953.108
-3.504055130D+08 2.083212387D+05-3.978209270D+01 5.039268720D-03-3.220707680D-07
 1.057379426D-11-1.396044154D-16                -1.662378721D+06 3.934491930D+02
CaO+              Gurvich,1996a pt1 p445 pt2 p351.
 3 tpis96 CA  1.00O   1.00E  -1.00    0.00    0.00 0   56.0768514     710237.542
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9163.110
 1.098060332D+05-1.459992448D+03 9.880777940D+00-9.157564600D-03 8.707582560D-06
-4.390411080D-09 9.264854660D-13                 9.150057350D+04-3.009947701D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9163.110
 9.397843130D+05-2.993362243D+03 8.336191820D+00-2.303295087D-03 7.373967530D-07
-1.052888279D-10 5.257138410D-15                 1.028098401D+05-2.461547836D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9163.110
-7.648645260D+07 1.739245253D+04 8.420288710D+00-1.168386844D-03 8.413684900D-08
-2.770799280D-12 3.569474430D-17                -8.643489770D+04-2.376513061D+01
CaOH              Gurvich,1996a pt1 p451 pt2 p355.
 2 tpis96 CA  1.00O   1.00H   1.00    0.00    0.00 0   57.0853400    -173307.350
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11049.697
 4.620028900D+04-9.285672820D+02 9.175828770D+00-3.962828800D-03 2.505447308D-06
 3.852068210D-11-3.352778470D-13                -1.798009717D+04-2.533704850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11049.697
 1.979972994D+06-5.598880990D+03 1.151348706D+01-1.668264707D-03 3.312573910D-07
-1.789056647D-11-3.580716410D-16                 1.340196822D+04-4.646084260D+01
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CaOH+              Gurvich,1996a pt1 p452 pt2 p356.
 2 tpis96 CA  1.00O   1.00H   1.00E  -1.00    0.00 0   57.0847914     372938.100
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11097.719
 4.884342660D+04-9.832415100D+02 9.610182950D+00-5.204360660D-03 4.263049820D-06
-1.197590878D-09 9.028411890D-15                 4.795056340D+04-2.827077334D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11097.719
 8.637615370D+05-2.347302046D+03 7.981911200D+00 1.003160947D-04-6.240074170D-08
 1.019540904D-11-5.698925280D-16                 5.830580120D+04-2.152181937D+01
Ca(OH)2            Gurvich,1996a pt1 p455 pt2 p358.
 2 tpis96 CA  1.00O   2.00H   2.00    0.00    0.00 0   74.0926800    -598338.869
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16592.281
 8.389257540D+04-1.791902135D+03 1.621891031D+01-7.840857170D-03 5.095111610D-06
-6.955487550D-11-6.132152640D-13                -6.600405630D+04-6.070913920D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16592.281
 1.721854884D+06-4.702217670D+03 1.396947691D+01 1.983791405D-04-1.243050592D-07
 2.033402404D-11-1.137157819D-15                -4.443761350D+04-5.287444860D+01
CaS                Gurvich,1996a pt1 p480 pt2 p374.
 2 tpis96 CA  1.00S   1.00    0.00    0.00    0.00 0   72.1430000     121475.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9360.113
 2.320990615D+04-4.518446080D+02 6.172333750D+00-3.598852020D-03 4.823731710D-06
-3.631733540D-09 1.212849867D-12                 1.554597691D+04-7.686936462D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9360.113
-1.568353214D+07 5.293855810D+04-6.322467240D+01 4.027726380D-02-1.114855081D-05
 1.464389344D-09-7.376078970D-14                -3.172022670D+05 4.799606012D+02
Ca2                Gurvich,1996a pt1 p439 pt2 p347.
 2 tpis96 CA  2.00    0.00    0.00    0.00    0.00 0   80.1560000     341765.336
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11273.136
-8.582228620D+04 1.588188960D+02 1.103952055D+01-3.333196760D-02 5.345938810D-05
-4.011573240D-08 1.160486682D-11                 3.770350800D+04-2.397744561D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11273.136
 2.405966267D+05 5.775803820D+01 2.347436675D+00 1.199275034D-04-4.329150310D-08
 7.015302690D-12-3.705660320D-16                 4.081875400D+04 1.895399607D+01
Cd                 Hf:Cox,1989. Moore,1971. Gordon,1999.
 3 g 7/97 CD  1.00    0.00    0.00    0.00    0.00 0  112.4110000     111800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.081751543D-04 1.816433041D-06 2.499999989D+00 3.129989231D-11-4.600710160D-14
 3.407048740D-17-9.989497436D-21                 1.270099766D+04 5.931549760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.699757467D+05 7.866001140D+02 1.628169079D+00 4.594123290D-04-1.150420443D-07
 1.074836707D-11 8.790199555D-17                 7.675148260D+03 1.220006052D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.336284287D+09 9.320949110D+05-2.490956222D+02 3.302878610D-02-2.200384347D-06
 7.425712550D-11-1.026730246D-15                -7.267528990D+06 2.167946107D+03
Cd+                Moore,1971. Gordon,1999.
 3 g 7/97 CD  1.00E  -1.00    0.00    0.00    0.00 0  112.4104514     985754.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21                 1.178129439D+05 6.624689450D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.484880812D+04-4.669153680D+01 2.557883006D+00-3.624701700D-05 1.213747570D-08
-2.072802814D-12 1.420665367D-16                 1.181070109D+05 6.216414480D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-6.428364400D+07 4.740395160D+04-1.165755517D+01 2.220273739D-03-1.964219980D-07
 9.262295070D-12-1.560026961D-16                -2.489244513D+05 1.263946278D+02
CL                 Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 7/97 CL  1.00    0.00    0.00    0.00    0.00 0   35.4530000     121301.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6271.588
 2.276215854D+04-2.168413293D+02 2.745185115D+00 2.451101694D-03-5.458011990D-06
 4.417986880D-09-1.288134004D-12                 1.501357068D+04 3.102963457D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6271.588
-1.697932930D+05 6.081726460D+02 2.128664090D+00 1.307367034D-04-2.644883596D-08
 2.842504775D-12-1.252911731D-16                 9.934387400D+03 8.844772103D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6271.588
-7.139687070D+07 4.499936330D+04-9.264315350D+00 1.657437964D-03-1.326219399D-07
 5.533998870D-12-8.390301878D-17                -3.405333030D+05 1.069111426D+02
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Appendix D (*continued*)

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CL+                Moore,1971. Moore,1970a. Gordon,1999.
 3 g 1/98 CL  1.00E  -1.00    0.00    0.00    0.00 0   35.4524514    1378799.635
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6386.335
 1.034697859D+05-1.293758873D+03 8.186702690D+00-9.916014600D-03 9.208472370D-06
-4.507426240D-09 9.182127880D-13                 1.714758780D+05-2.766417931D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6386.335
 4.056409480D+04-4.960165720D+01 3.101653630D+00-5.868738290D-04 2.252039316D-07
-3.299703020D-11 1.708780842D-15                 1.652982337D+05 2.574942598D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6386.335
-3.078099946D+06-6.858418280D+02 3.092289282D+00-1.922260015D-05 3.805551560D-10
-1.571848967D-13 8.442513880D-18                 1.683434405D+05 1.334407234D+00
CL-                Hotop,1985. Gordon,1999.
 3 g 4/97 CL  1.00E   1.00    0.00    0.00    0.00 0   35.4535486    -233957.972
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.888389093D+04 4.200642023D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.888389093D+04 4.200642023D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.888389093D+04 4.200642023D+00
CLCN               Gurvich,1991 pt1 p230 pt2 p218
 2 g 6/95 CL  1.00C   1.00N   1.00    0.00    0.00 0   61.4704000     134200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10669.042
 7.274043430D+04-1.297344947D+03 1.107676527D+01-1.108430216D-02 1.614009477D-05
-1.088916772D-08 2.830952246D-12                 2.084388986D+04-3.597370046D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10669.042
 3.467573120D+05-1.957857370D+03 8.807806150D+00-4.388362780D-04 1.024761895D-07
-1.110675026D-11 4.986179420D-16                 2.581923944D+04-2.636885363D+01
CLF                Gurvich,1989 pt1 p190 pt2 p97.
 2 tpis89 CL  1.00F   1.00    0.00    0.00    0.00 0   54.4514032     -55700.993
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8908.107
 3.352210810D+04-3.688311900D+02 4.272288620D+00 2.549434508D-03-4.456830890D-06
 3.413854120D-09-9.838685200D-13                -5.839369690D+03 2.318014199D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8908.107
 3.045867173D+06-9.979328260D+03 1.684162254D+01-7.465850620D-03 2.336213612D-06
-3.365865460D-10 1.763082415D-14                 5.447120800D+04-8.707987094D+01
CLF3               Gurvich,1989 pt1 p193 pt2 p98.
 2 tpis89 CL  1.00F   3.00    0.00    0.00    0.00 0   92.4482096    -164600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13728.449
 1.285175171D+05-2.140445721D+03 1.493096474D+01-6.042471040D-03 3.718968610D-06
-8.053201100D-10-7.985600530D-14                -1.138459640D+04-5.594838353D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13728.449
-2.294956235D+05-1.220741000D+02 1.009124644D+01-3.649724750D-05 8.058910750D-09
-9.230849950D-13 4.272569490D-17                -2.282840447D+04-2.511605479D+01
CLF5               Gurvich,1989 pt1 p194 pt2 p99.
 2 tpis89 CL  1.00F   5.00    0.00    0.00    0.00 0  130.4450160    -238000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17930.396
 2.459703939D+05-4.315348070D+03 2.727005972D+01-1.670193839D-02 1.421668208D-05
-6.426479740D-09 1.183099799D-12                -1.071423726D+04-1.267466837D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17930.396
-4.269327450D+05-2.058057390D+02 1.615465278D+01-6.212688180D-05 1.376637959D-08
-1.581335709D-12 7.336422490D-17                -3.361466600D+04-5.757531175D+01
CLO                Gurvich,1989 pt1 p180 pt2 p90.
 2 tpis89 CL  1.00O   1.00    0.00    0.00    0.00 0   51.4524000     101621.115
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9522.115
-1.687268145D+04 2.573812247D+02 2.175846120D+00 6.432061130D-03-8.568249500D-06
 5.764971250D-09-1.545771209D-12                 9.829518980D+03 1.386010503D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9522.115
 4.093760520D+05-1.765985112D+03 7.087900630D+00-1.828450169D-03 7.103818100D-07
-1.209332942D-10 7.076441040D-15                 2.151891784D+04-1.668645548D+01
CLO2               Gurvich,1989 pt1 p182 pt2 p91.
 2 g 7/93 CL  1.00O   2.00    0.00    0.00    0.00 0   67.4518000     105000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10800.646
-1.127277696D+04 3.903032030D+02-3.843018530D-01 2.108677947D-02-2.793137755D-05
 1.841289286D-08-4.839779150D-12                 9.756933670D+03 2.913262700D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10800.646
-1.633793802D+05-3.161480670D+02 7.009787260D+00 2.837971144D-04-1.179925338D-07
 2.920383252D-11-2.024030202D-15                 1.184946452D+04-1.091168827D+01
```

Appendix D (*continued*)

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CL2               Ref-Elm. Gurvich,1989 pt1 p177 pt2 p88.
 2 tpis89 CL  2.00    0.00    0.00    0.00    0.00 0   70.9060000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9181.110
 3.462815170D+04-5.547126520D+02 6.207589370D+00-2.989632078D-03 3.173027290D-06
-1.793629562D-09 4.260043590D-13                 1.534069331D+03-9.438331107D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9181.110
 6.092569420D+06-1.949627662D+04 2.854535795D+01-1.449968764D-02 4.463890770D-06
-6.358525860D-10 3.327360290D-14                 1.212117724D+05-1.690778824D+02
CL2O              Gurvich,1989 pt1 p184 pt2 p92.
 2 tpis89 CL  2.000   1.00    0.00    0.00    0.00 0   86.9054000       79000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11695.482
 7.798855400D+04-1.182537879D+03 9.526514660D+00-2.596163176D-03 8.696781310D-07
 4.484098270D-10-3.044511967D-13                 1.376729572D+04-2.484690718D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11695.482
-1.271743461D+05-6.741963220D+01 7.050022450D+00-1.988084386D-05 4.366209050D-09
-4.978580680D-13 2.295679186D-17                 7.387289300D+03-8.797477254D+00
Co                Hf:Hultgren,1973. Sugar,1985. Gordon,1999.
 3 g 7/97 CO  1.00    0.00    0.00    0.00    0.00 0   58.9332000      428441.600
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6359.768
-2.598939184D+03 2.461989844D+02-6.106058370D-01 1.393005772D-02-2.210012979D-05
 1.623755261D-08-4.534904351D-12                 4.984613760D+04 2.257584199D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6359.768
 1.381841305D+06-3.756036680D+03 6.657130650D+00-1.269246675D-03 1.464092329D-07
 6.574946570D-12-1.102384178D-15                 7.494442910D+04-2.258500836D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6359.768
-5.468015750D+08 4.037704950D+05-1.142413163D+02 1.663014422D-02-1.156228007D-06
 3.862515150D-11-5.002032746D-16                -3.076031798D+06 1.003028648D+03
Co+               Sugar,1985. Gordon,1999.
 3 g 7/97 CO  1.00E -1.00    0.00    0.00    0.00 0   58.9326514     1193003.307
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6291.507
 1.028494160D+05-8.744731260D+02 4.279500280D+00 2.225857835D-03-7.457274570D-06
 7.279221950D-09-2.347541963D-12                 1.474895959D+05-5.679019220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6291.507
 2.907386174D+06-8.619705750D+03 1.188134934D+01-3.510647420D-03 5.748004680D-07
-2.534065135D-11 2.976607469D-16                 1.977419221D+05-6.096533440D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6291.507
 2.701785479D+09-1.604232092D+06 3.687314770D+02-4.041150820D-02 2.371848586D-06
-7.119952160D-11 8.635423717D-16                 1.293631390D+07-3.201662470D+03
Co-               Hotop,1985. Gordon,1999.
 3 g 9/97 CO  1.00E  1.00    0.00    0.00    0.00 0   58.9337486      358414.372
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6306.772
 3.459493760D+04-1.355041712D+02 1.116330898D+00 9.042761830D-03-1.454296726D-05
 9.994940630D-09-2.595633259D-12                 4.337037820D+04 1.270494975D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6306.772
-5.741394170D+05 1.763109207D+03 1.415561988D+00 3.776869690D-04-7.534179980D-08
 7.995701540D-12-3.490440000D-16                 3.083493114D+04 1.634360353D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6306.772
-7.121795840D+05 7.962447120D+02 2.328870839D+00 1.919463732D-05-1.179708474D-09
 3.764228600D-14-4.875340940D-19                 3.689285080D+04 9.511282720D+00
Cr                Hf:Chase,1998 p963 6/79. Sugar,1985. Gordon,1999.
 3 g 7/97 CR  1.00    0.00    0.00    0.00    0.00 0   51.9961000      397480.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.335658217D+03-2.102424026D+01 2.631908173D+00-4.246263250D-04 7.439194160D-07
-6.763931630D-10 2.507855625D-13                 4.715866640D+04 6.005425450D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.120220789D+07 3.401163690D+04-3.657062170D+01 2.110296902D-02-5.518180140D-06
 7.173601710D-10-3.505127367D-14                -1.688993440D+05 2.864481267D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 3.900886930D+09-2.462918543D+06 5.915632640D+02-6.697121640D-02 3.946957790D-06
-1.166504597D-10 1.367279456D-15                 1.955381984D+07-5.133510550D+03
Cr+               Sugar,1985. Gordon,1999.
 3 g 7/97 CR  1.00E -1.00    0.00    0.00    0.00 0   51.9955514     1056546.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.819187467D+02-2.188843517D+00 2.510676511D+00-2.706791825D-05 3.768492630D-08
-2.736784742D-11 8.115389932D-15                 1.263380825D+05 6.506276170D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 3.342330790D+06-1.064261051D+04 1.557884307D+01-7.708971480D-03 2.158300274D-06
-2.368108110D-10 8.952805604D-15                 1.932997670D+05-8.604356670D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.853867040D+08-4.114535830D+05 1.242898882D+02-1.610102894D-02 1.147677369D-06
-4.099673600D-11 5.728606039D-16                 3.281645810D+06-1.034723629D+03
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Cr-                Hotop,1985. Gordon,1999.
 3 g10/97 CR  1.00E   1.00     0.00     0.00     0.00 0   51.9966486      327023.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.858627870D+04 6.566835370D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.858627870D+04 6.566835370D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.858627870D+04 6.566835370D+00
CrN                Chase,1998 p967.
 2 j12/73 CR  1.00N   1.00     0.00     0.00     0.00 0   66.0028000      505008.800
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8777.789
-8.239129220D+03 3.008144202D+02 5.147874920D-01 1.129636791D-02-1.515183504D-05
 1.010997229D-08-2.687775750D-12                 5.845628120D+04 2.298028696D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8777.789
 1.110672490D+06-3.690478540D+03 8.599056680D+00-2.125587223D-03 5.282358480D-07
-4.921139150D-11 1.404331106D-15                 8.254804580D+04-2.799968411D+01
CrO                Gurvich,1982 pt1 p13 pt2 p17.
 3 tpis82 CR  1.00O   1.00     0.00     0.00     0.00 0   67.9955000      186581.318
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9849.118
 9.373334110D+03 1.369743818D+02 1.621443428D+00 8.814095960D-03-1.232845360D-05
 8.497960940D-09-2.315804197D-12                 2.090948871D+04 1.781935787D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9849.118
 1.092367332D+06-3.749758650D+03 9.007870210D+00-2.545445236D-03 6.928051680D-07
-6.390831950D-11 1.659741645D-15                 4.447098210D+04-2.942600453D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9849.118
 5.600191720D+08-3.409592350D+05 7.971428300D+01-7.045904880D-03 3.311256200D-07
-8.196877430D-12 8.487479810D-17                 2.738393714D+06-6.629641700D+02
CrO2               Gurvich,1982 pt1 p16 pt2 p19.
 2 tpis82 CR  1.00O   2.00     0.00     0.00     0.00 0   83.9949000     -108043.235
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10693.869
 3.548629900D+04-2.298628537D+02 2.286289393D+00 1.616929338D-02-2.345198910D-05
 1.631365714D-08-4.444269620D-12                -1.278912840D+04 1.442954956D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10693.869
-4.327109140D+05 1.915584657D+02 7.188247370D+00-5.694846190D-04 3.546366130D-07
-5.655123060D-11 2.908946349D-15                -1.743339545D+04-1.006424720D+01
CrO3               Gurvich,1982 pt1 p17 pt2 p20.
 2 tpis82 CR  1.00O   3.00     0.00     0.00     0.00 0   99.9943000     -322037.084
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13040.072
 4.183020060D+04-5.059348850D+02 4.432715670D+00 1.995079387D-02-2.920597649D-05
 2.039330280D-08-5.580086630D-12                -3.769702400D+04 8.653827280D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13040.072
-6.283314010D+05 6.928158180D+02 8.971274600D+00 6.823365640D-04-2.235048825D-07
 3.366785790D-11-1.614026492D-15                -4.723880200D+04-1.945305345D+01
CrO3-              Gurvich,1982 pt1 p18 pt2 p21.
 2 tpis82 CR  1.00O   3.00E   1.00     0.00     0.00 0   99.9948486     -632850.845
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13423.739
 1.873455703D+05-2.300722991D+03 1.343953022D+01-1.663085846D-03-1.443973096D-06
 2.045898933D-09-6.837555300D-13                -6.630111580D+04-4.930644200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13423.739
-6.499682030D+05 4.522017620D+02 9.980575900D+00-4.214136730D-04 2.631277945D-07
-4.594543650D-11 2.659097549D-15                -8.350019730D+04-2.464810900D+01
Cs                 Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 7/97 CS  1.00     0.00     0.00     0.00     0.00 0  132.9054500       76500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 5.466584070D+01-8.279346040D-01 2.504942210D+00-1.494620690D-05 2.425976774D-08
-2.013172322D-11 6.704271991D-15                 8.459321390D+03 6.848825772D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 6.166040900D+06-1.896175522D+04 2.483229903D+01-1.251977234D-02 3.309017390D-06
-3.354012020D-10 9.626500908D-15                 1.285111231D+05-1.522942188D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-9.566231720D+08 4.321690420D+05-6.371801020D+01 5.246260580D-03-2.366560159D-07
 5.848488480D-12-6.169370441D-17                -3.585268840D+06 6.156618174D+02
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Cs+                Moore,1971. Gordon,1999.
 3 g 1/98 CS  1.00E  -1.00     0.00     0.00     0.00 0  132.9049014      458401.828
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.438737820D+04 6.182757992D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.438737820D+04 6.182757992D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.479469300D+08 1.405115456D+05-2.805027359D+01 3.087928133D-03-1.273598265D-07
-3.748818380D-13 1.214944533D-16                -1.072498017D+06 2.756827325D+02
Cs-                Hotop,1985. Gordon,1999.
 3 g10/97 CS  1.00E   1.00     0.00     0.00     0.00 0  132.9059986      24797.228
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.237029001D+03 6.182770382D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.237029001D+03 6.182770382D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.237029001D+03 6.182770382D+00
CsBO2              Gurvich,1982 pt1 p505 pt2 p526.
 2 tpis82 CS  1.00B   1.00O   2.00     0.00     0.00 0  175.7152500     -686901.906
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14466.094
 4.193609580D+04-6.664237400D+02 8.134835880D+00 2.902960302D-03-7.881467920D-07
-8.327694540D-10 4.441719110D-13                -8.122320070D+04-1.121622595D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14466.094
 8.975579890D+04-1.656134283D+03 1.116468934D+01-4.476366990D-04 9.621091810D-08
-1.081470115D-11 4.938446740D-16                -7.610479670D+04-3.036616012D+01
CsBr               Gurvich,1982 pt1 p490 pt2 p512.
 2 tpis82 CS  1.00BR  1.00     0.00     0.00     0.00 0  212.8094500     -206828.875
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10406.125
 1.639263647D+03-6.947477970D+01 4.860058720D+00-8.587780150D-04 1.375177550D-06
-9.891766980D-10 2.895433432D-13                -2.589550471D+04 4.465355690D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10406.125
-1.528329963D+05 1.259712657D+03 1.704268408D+00 2.776255318D-03-1.228389838D-06
 2.698111786D-10-1.983534480D-14                -3.327842030D+04 2.484116659D+01
CsCL               Gurvich,1982 pt1 p487 pt2 p509.
 2 tpis82 CS  1.00CL  1.00     0.00     0.00     0.00 0  168.3584500     -242228.878
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10131.122
-2.538165292D+04 2.972839326D+02 2.667813848D+00 5.583272410D-03-8.529005090D-06
 6.595191390D-09-1.989715823D-12                -3.189251450D+04 1.511365709D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10131.122
-3.674923480D+06 1.186152941D+04-1.063287842D+01 9.804117920D-03-3.277797460D-06
 5.534233390D-10-3.401231500D-14                -1.048658658D+05 1.114096064D+02
CsF                Gurvich,1982 pt1 p483 pt2 p506.
 2 tpis82 CS  1.00F   1.00     0.00     0.00     0.00 0  151.9038532     -364214.884
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9645.116
 1.843685799D+04-4.042409390D+02 6.383178860D+00-4.674323370D-03 6.630134010D-06
-4.760905530D-09 1.374569797D-12                -4.318489590D+04-7.226593230D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9645.116
-1.850863231D+06 5.625298800D+03-2.250022212D+00 4.109243540D-03-1.250243837D-06
 1.941483152D-10-1.071166179D-14                -8.079827790D+04 5.135559450D+01
CsH                Gurvich,1982 pt1 p477 pt2 p501.
 2 tpis82 CS  1.00H   1.00     0.00     0.00     0.00 0  133.9133900      115950.106
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8846.106
 1.620544411D+04-7.087016280D+01 2.480847135D+00 7.021985990D-03-1.007126309D-05
 7.090639030D-09-1.950395735D-12                 1.342777328D+04 9.894247170D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8846.106
-9.112146650D+05 3.576472750D+03-1.258058765D+00 4.314855150D-03-1.407820502D-06
 2.154598897D-10-1.254525606D-14                -9.158717270D+03 3.908800030D+01
CsI                Gurvich,1982 pt1 p494 pt2 p515.
 2 tpis82 CS  1.00I   1.00     0.00     0.00     0.00 0  259.8099200     -152319.873
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10550.127
-4.072685650D+03 2.330073667D+01 4.387277690D+00 3.412084290D-04-2.175588153D-07
 8.906787000D-11-2.182639837D-15                -1.978766885D+04 8.074657820D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10550.127
 4.511259050D+06-1.341706362D+04 1.980984712D+01-8.359855550D-03 2.348201245D-06
-2.874285248D-10 1.208087750D-14                 6.573439130D+04-1.021032592D+02
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CsLi              Gurvich,1982 pt1 p505 pt2 p527.
 2 tpis82 CS  1.00LI  1.00    0.00    0.00    0.00 0  139.8464500     162146.324
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10341.124
 1.368709568D+03-7.451297060D+01 4.845620930D+00-5.573667210D-04 4.953326760D-07
 4.369068910D-10-4.608145770D-13                 1.850577392D+04 2.112012017D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10341.124
 7.481630230D+06-2.885297839D+04 4.631104990D+01-2.784288108D-02 8.787413490D-06
-1.264901197D-09 6.720186280D-14                 1.945137819D+05-2.857846194D+02
CsNO2             Gurvich,1982 pt1 p499 pt2 p520.
 2 tpis82 CS  1.00N   1.00O   2.00    0.00    0.00 0  178.9109500    -210339.828
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15980.172
-7.106010440D+04 1.272448257D+03-2.447362349D+00 3.064441948D-02-3.699225940D-05
 2.259121812D-08-5.580635910D-12                -3.313370920D+04 4.954693336D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15980.172
-1.633503154D+05-8.468879580D+02 1.062853461D+01-2.508799215D-04 5.541255770D-08
-6.355591950D-12 2.946880031D-16                -2.403040739D+04-2.443488888D+01
CsNO3             Gurvich,1982 pt1 p501 pt2 p522.
 2 tpis82 CS  1.00N   1.00O   3.00    0.00    0.00 0  194.9103500    -318486.390
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16563.610
-2.677219779D+04 9.011692690D+02-3.265340820D+00 4.298377700D-02-5.386751380D-05
 3.384527520D-08-8.565223660D-12                -4.405304140D+04 5.118862689D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16563.610
-3.147517676D+05-1.367011655D+03 1.401012848D+01-4.018647130D-04 8.853614700D-08
-1.013466457D-11 4.691758730D-16                -3.549026670D+04-4.500692791D+01
CsNa              Gurvich,1982 pt1 p506 pt2 p528.
 2 tpis82 CS  1.00NA  1.00    0.00    0.00    0.00 0  155.8952200     125907.329
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10702.129
 2.521738609D+04-4.295362490D+02 7.223094740D+00-8.460463000D-03 1.443905157D-05
-1.143624855D-08 3.183721930D-12                 1.579099265D+04-8.838790300D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10702.129
 3.879556790D+06-1.780167288D+04 3.491355800D+01-2.320080793D-02 7.861975840D-06
-1.171011257D-09 6.323927370D-14                 1.195776556D+05-2.001754433D+02
CsO               Gurvich,1982 pt1 p471 pt2 p493.
 2 tpis82 CS  1.00O   1.00    0.00    0.00    0.00 0  148.9048500      37587.318
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9835.118
 8.683958810D+03 4.250278170D+02-3.484055300D+00 3.801969830D-02-6.651927560D-05
 5.173472190D-08-1.512567066D-11                 1.969690015D+03 4.240796140D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9835.118
 8.375544350D+05-2.418205772D+03 8.908065350D+00-3.378180040D-03 1.312755917D-06
-2.150508925D-10 1.219138980D-14                 1.809493447D+04-2.460858580D+01
CsOH              Gurvich,1997.
 2 g 9/97 CS  1.00O   1.00H   1.00    0.00    0.00 0  149.9127900    -256000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11834.689
 9.386960790D+03-5.009354260D+02 8.301351980D+00-3.235596840D-03 2.612406777D-06
-4.950613410D-10-1.038364927D-13                -3.025722427D+04-1.742194837D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11834.689
 8.967171130D+05-2.323978587D+03 7.959644870D+00 1.101149275D-04-6.466013970D-08
 1.045968201D-11-5.822514170D-16                -1.736258234D+04-1.864239624D+01
CsRb              Gurvich,1982 pt1 p508 pt2 p530.
 2 tpis82 CS  1.00RB  1.00    0.00    0.00    0.00 0  218.3732500     111477.332
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10972.132
-4.910922680D+03-9.209015550D+00 5.193377890D+00-4.390246990D-03 1.254790436D-05
-1.414878514D-08 5.101441310D-12                 1.200498171D+04 5.361542930D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10972.132
-1.328693378D+07 3.414579470D+04-2.373696406D+01 7.070465400D-03 3.863450970D-07
-3.158132986D-10 2.667747207D-14                -2.124008997D+05 2.239970251D+02
Cs2               Gurvich,1982 pt1 p467 pt2 p492.
 2 tpis82 CS  2.00    0.00    0.00    0.00    0.00 0  265.8109000     109404.333
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11029.133
-4.674158730D+04 5.952019510D+02 1.895333975D+00 4.082065810D-03 2.531487119D-06
-9.085139030D-09 4.290179930D-12                 8.857282570D+03 2.391592727D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11029.133
-2.592739590D+07 7.539818910D+04-7.484086800D+01 3.692866790D-02-8.082497240D-06
 8.171850730D-10-3.089285900D-14                -4.715045720D+05 5.860933750D+02
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Cs2Br2            Gurvich,1982 pt1 p491 pt2 p513.
 2 tpis82 CS  2.00BR  2.00    0.00    0.00    0.00 0  425.6189000    -565828.869
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22113.130
-6.321285180D+03-1.213153529D+01 1.004967112D+01-1.102100044D-04 1.365293456D-07
-8.856957070D-11 2.339447704D-14                -7.099771710D+04-7.539424790D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22113.130
-7.545846650D+03-2.087093009D-01 1.000018042D+01-8.034260730D-08 1.923604258D-11
-2.344698140D-15 1.139365834D-19                -7.105883540D+04-7.251793040D+00
Cs2CO3            Gurvich,1982 pt1 p503 pt2 p524.
 2 tpis82 CS  2.00C   1.00O   3.00    0.00    0.00 0  325.8198000    -806447.939
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21179.061
-4.673130000D+04 9.436549060D+02-2.374670436D-01 4.168484610D-02-5.094372210D-05
 3.132078394D-08-7.780421670D-12                -1.039162411D+05 4.055853980D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21179.061
-3.037149985D+05-1.517078400D+03 1.711941656D+01-4.449700120D-04 9.798325240D-08
-1.121256063D-11 5.189734780D-16                -9.420414770D+04-5.682006260D+01
Cs2CL2            Gurvich,1982 pt1 p487 pt2 p510.
 2 tpis82 CS  2.00CL  2.00    0.00    0.00    0.00 0  336.7169000    -644658.398
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20944.712
-1.077956357D+04-5.346106950D+01 1.021710683D+01-4.789687030D-04 5.908946530D-07
-3.821416520D-10 1.006995985D-13                -8.029515170D+04-1.207856486D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20944.712
-1.625143966D+04-9.006137350D-01 1.000077173D+01-3.416194080D-07 8.144968080D-11
-9.897475280D-15 4.798330810D-19                -8.056513220D+04-1.081977337D+01
Cs2F2             Gurvich,1982 pt1 p484 pt2 p507.
 2 tpis82 CS  2.00F   2.00    0.00    0.00    0.00 0  303.8077064    -891858.506
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19388.600
-9.942677480D+03-2.536723355D+02 1.100684073D+01-2.185640152D-03 2.664791874D-06
-1.708229209D-09 4.471151980D-13                -1.090582601D+05-2.000699602D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19388.600
-3.677946420D+04-4.355753480D+00 1.000366687D+01-1.603814186D-06 3.791469740D-10
-4.578687430D-14 2.209385787D-18                -1.103456448D+05-1.415086452D+01
Cs2I2             Gurvich,1982 pt1 p495 pt2 p516.
 2 tpis82 CS  2.00I   2.00    0.00    0.00    0.00 0  519.6198400    -454033.097
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22584.903
-4.449286970D+03-5.321793660D+00 1.002183919D+01-4.853374850D-05 6.019338400D-08
-3.908226390D-11 1.032981014D-14                -5.757823380D+04-5.271267090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22584.903
-4.983376010D+03-9.461179880D-02 1.000008229D+01-3.680962040D-08 8.844660910D-12
-1.081178562D-15 5.266141980D-20                -5.760501040D+04-5.144864890D+00
Cs2O              Gurvich,1982 pt1 p473 pt2 p496.
 2 tpis82 CS  2.00O   1.00    0.00    0.00    0.00 0  281.8103000    -142855.345
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14089.855
 1.910533804D+04-4.962181530D+02 8.759606300D+00-3.511622790D-03 4.016479830D-06
-2.450899853D-09 6.172404890D-13                -1.677664956D+04-1.159258822D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14089.855
-4.119147410D+04-1.079255391D+01 7.008500470D+00-3.542955780D-06 8.081699120D-10
-9.499419930D-14 4.489122540D-18                -1.934377850D+04-1.203970450D+00
Cs2O+             Gurvich,1982 pt1 p474 pt2 p497.
 2 tpis82 CS  2.00O   1.00E  -1.00    0.00    0.00 0  281.8097514     283699.926
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14447.726
 6.837056090D+02-2.435575007D+02 7.783037470D+00-1.414552725D-03 1.470799739D-06
-8.218821330D-10 1.911749489D-13                 3.324194870D+04-4.750423560D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14447.726
-3.153085844D+04-5.771559030D+00 7.004482630D+00-1.848241331D-06 4.180882300D-10
-4.882376270D-14 2.295419936D-18                 3.196227310D+04-5.434350690D-02
Cs2O2             Gurvich,1982 pt1 p476 pt2 p499.
 2 tpis82 CS  2.00O   2.00    0.00    0.00    0.00 0  297.8097000    -247069.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17426.496
 2.274505180D+04-5.667912570D+02 1.001728332D+01 2.547081016D-03-4.909216690D-06
 3.848788910D-09-1.124566008D-12                -2.947334360D+04-1.841275291D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17426.496
-1.190032094D+05-9.261075260D+01 1.006915777D+01-2.766227147D-05 6.110752960D-09
-7.003595480D-13 3.243742520D-17                -3.255610740D+04-1.724868948D+01
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Cs2O2H2           Gurvich,1997.
 2 g 9/97 CS  2.00O   2.00H   2.00    0.00    0.00 0  299.8255800    -653000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23937.353
-1.085981041D+04-6.883068420D+02 1.643543354D+01-4.039220580D-03 2.331117156D-06
 8.439651630D-10-6.859309730D-13                 -7.939476230D+04-4.906196810D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23937.353
 1.802857941D+06-4.656354750D+03 1.693566597D+01 2.117402535D-04-1.272249096D-07
 2.066555839D-11-1.152390667D-15                 -5.190813690D+04-5.849719160D+01
Cs2SO4            Gurvich,1982 pt1 p497 pt2 p518.
 2 g10/99 CS  2.00S   1.000   4.00    0.00    0.00 0  361.8735000   -1117651.834
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23988.166
 6.153637870D+04-6.381374330D+02 6.894772090D+00 3.960182910D-02-5.529862010D-05
 3.736332520D-08-9.973241830D-12                 -1.339760310D+05-1.284432588D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23988.166
-5.223397520D+05-9.444155250D+02 1.970476453D+01-2.821225990D-04 6.240792280D-08
-7.163464070D-12 3.322667190D-16                 -1.364179983D+05-6.820406795D+01
Cu                Hf:Cox,1989. Sugar,1990. Gordon,1999.
 3 g12/97 CU  1.00    0.00    0.00    0.00    0.00 0   63.5460000     337400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 7.713133150D+01-1.169236206D+00 2.506987803D+00-2.116434879D-05 3.441714710D-08
-2.862608999D-11 9.559250991D-15                  3.983981210D+04 5.730813220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.308090411D+06-8.503261000D+03 1.467859102D+01-8.467136520D-03 2.887821016D-06
-4.270659180D-10 2.304265084D-14                  9.207535620D+04-7.854701560D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-6.490595890D+08 4.240323360D+05-1.028965806D+02 1.297259934D-02-7.766697680D-07
 2.220446727D-11-2.441532031D-16                 -3.305304580D+06 9.198622920D+02
Cu+               Sugar,1990. Gordon,1999.
 3 g 3/98 CU  1.00E  -1.00    0.00    0.00    0.00 0   63.5454514    1089079.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.452340093D-03 2.606893531D-05 2.499999890D+00 2.351922485D-10-2.669362382D-13
 1.510315123D-16-3.278224814D-20                  1.302400621D+05 5.075940770D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.181443016D+06 7.217858190D+03-6.941154750D+00 6.208248920D-03-2.139340497D-06
 3.566431440D-10-2.081198501D-14                  8.516456660D+04 7.116800670D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.994686480D+09-1.831416099D+06 4.294926960D+02-4.801927720D-02 2.836504248D-06
-8.452189040D-11 1.013018211D-15                  1.468809255D+07-3.729918010D+03
Cu-               Hotop,1985. Gordon,1999.
 3 g10/97 CU  1.00E   1.00    0.00    0.00    0.00 0   63.5465486     212718.628
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  2.483864954D+04 5.075966030D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  2.483864954D+04 5.075966030D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  2.483864954D+04 5.075966030D+00
CuCL              Chase,1998 p748.
 2 j 3/66 CU  1.00CL  1.00    0.00    0.00    0.00 0   98.9990000      91090.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9471.175
 1.469847736D+04-3.393167250D+02 5.723459590D+00-2.417296132D-03 2.858019864D-06
-1.757900548D-09 4.455047290D-13                  1.131714015D+04-4.527352594D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9471.175
-2.577122410D+04-7.106346060D+00 4.505623180D+00 5.394548270D-05 5.386417960D-10
-6.348482770D-14 3.006622062D-18                  9.566192870D+03 2.680067564D+00
CuF               Chase,1998 p1013.
 2 j12/77 CU  1.00F   1.00    0.00    0.00    0.00 0   82.5444032     -12550.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9083.091
 3.761385410D+04-5.468104900D+02 5.832351720D+00-1.695312068D-03 1.218150880D-06
-3.713285280D-10 2.002276589D-14                  5.865140720D+01-7.156930090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9083.091
 5.094154830D+05-1.415009870D+03 5.632349380D+00-1.629128410D-04-1.156611499D-07
 5.066034080D-11-4.153205110D-15                  6.305506600D+03-7.407773610D+00
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Appendix D (*continued*)

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CuF2              Chase,1998 p1017.
 2 j12/77 CU  1.00F   2.00     0.00     0.00     0.00 0  101.5428064     -266940.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12055.910
 6.573311280D+04-8.962430840D+02 7.917560940D+00 1.345667904D-03-4.162400010D-06
 3.716181090D-09-1.155537597D-12                 -2.916887325D+04-1.587076153D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12055.910
-1.650355082D+06 3.775362120D+03 3.889116550D+00 6.821912640D-04 1.875979026D-07
-5.677368110D-11 3.823248730D-15                 -5.953371700D+04 1.522659664D+01
CuO               Chase,1998 p1020.
 2 j12/77 CU  1.00O   1.00     0.00     0.00     0.00 0   79.5454000      306270.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9750.939
 4.689762240D+03-1.184808464D+02 4.566155240D+00 4.309058020D-04-8.309886400D-07
 6.946638020D-10-2.108693366D-13                  3.615190680D+04 1.733847344D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9750.939
 3.582280170D+05-9.139366410D+02 5.136898670D+00 6.240577240D-05-1.558613495D-07
 5.236803120D-11-4.026745620D-15                  4.150792860D+04-2.634070960D+00
Cu2               Chase,1998 p1022.
 2 j 9/66 CU  2.00    0.00     0.00     0.00     0.00 0  127.0920000      485340.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9930.154
-8.529183480D+02-9.720044930D+01 4.882233700D+00-7.371369400D-04 1.000575401D-06
-6.391989440D-10 1.668655797D-13                  5.749307020D+04 1.105391325D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9930.154
-8.699399500D+04 3.209103870D+02 3.973802880D+00 5.080809670D-04-1.707470385D-07
 3.219108190D-11-1.958830868D-15                  5.506090190D+04 6.914502170D+00
Cu3CL3            Chase,1998 p874.
 2 j 3/66 CU  3.00CL  3.00     0.00     0.00     0.00 0  296.9970000     -258570.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          28723.690
 4.487885320D+03-8.736644440D+02 1.936189091D+01-7.137447860D-03 8.560454870D-06
-5.419978740D-09 1.405175350D-12                 -3.162689960D+04-5.976797945D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          28723.690
-9.188559680D+04-1.571936430D+01 1.601294170D+01-5.572992370D-06 1.302748507D-09
-1.560175322D-13 7.480827570D-18                 -3.608760740D+04-4.013211395D+01
D                 D0(D2): Herzberg,1970. Moore,1972. Gordon,1999.
 3 g 6/97 D   1.00    0.00     0.00     0.00     0.00 0    2.0141020      221720.228
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  2.592128700D+04 5.917143380D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 6.050019210D+01-1.810766064D-01 2.500210817D+00-1.220711706D-07 3.715172170D-11
-5.660680210D-15 3.393920393D-19                  2.592243752D+04 5.902125370D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 2.169259778D+08-1.309309862D+05 3.392595050D+01-3.805973810D-03 2.427699393D-07
-7.677967800D-12 9.624191177D-17                  1.065922040D+06-2.726201602D+02
D+                Moore,1972. Gordon,1999.
 3 g 9/96 D   1.00E  -1.00     0.00     0.00     0.00 0    2.0135534     1540324.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  1.845120037D+05-1.018414521D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  1.845120037D+05-1.018414521D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  1.845120037D+05-1.018414521D-01
D-                Hotop,1985. Gordon,1999.
 3 g 8/96 D   1.00E   1.00     0.00     0.00     0.00 0    2.0146506      142752.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  1.642373393D+04-1.010243437D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  1.642373393D+04-1.010243437D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  1.642373393D+04-1.010243437D-01
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DBr                Gurvich,1989 pt1 p206 pt2 p107.
 2 tpis89 D   1.00BR  1.00    0.00    0.00    0.00 0   81.9181020      -37036.496
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8668.104
-1.918282458D+04 2.020175399D+02 3.044629038D+00-1.488157450D-03 6.870897800D-06
-6.591160280D-09 2.093769216D-12                 -6.560074400D+03 8.008690040D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8668.104
 6.654000440D+05-2.594092228D+03 6.885879400D+00-1.103284901D-03 2.894201105D-07
-3.152037514D-11 1.011011776D-15                  1.037813140D+04-1.973703653D+01
DCL                Gurvich,1989 pt1 p188 pt2 p95.
 2 tpis89 D   1.00CL  1.00    0.00    0.00    0.00 0   37.4671020      -93547.003
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8661.104
 1.046421033D+04-2.313813446D+02 5.420693260D+00-7.508012650D-03 1.398672495D-05
-1.066249569D-08 3.011167635D-12                 -1.128403374D+04-6.711842349D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8661.104
 4.117284900D+05-1.764535217D+03 5.668877100D+00-3.475964170D-04 5.882688030D-08
 3.760253130D-13-5.164600560D-16                 -1.541258092D+03-1.275659404D+01
DF                 Gurvich,1989 pt1 p172 pt2 p80.
 3 tpis89 D   1.00F   1.00    0.00    0.00    0.00 0   21.0125052      -276227.596
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8638.104
 5.721370750D+04-7.311733800D+02 7.220870870D+00-9.423969350D-03 1.208025139D-05
-6.941812690D-09 1.538525476D-12                 -3.069230024D+04-1.932760992D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8638.104
 8.001172800D+05-2.438386832D+03 5.620664450D+00-2.020416838D-04 1.714418979D-08
 2.697462563D-12-2.888297410D-16                 -1.857447029D+04-1.473004444D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8638.104
 1.924190104D+08-9.333761700D+04 1.929651319D+01-6.429319300D-04-1.978551386D-08
 1.730048706D-12-3.030499069D-17                  7.325924600D+05-1.428958225D+02
DOCL               D0 estimated from HOCL. Jacox,1998 p155.
 2 g 1/01 D   1.00O   1.00CL  1.00    0.00    0.00 0   53.4665020      -79538.686
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10324.814
 6.852834290D+04-7.673444550D+02 5.933970140D+00 2.868820667D-03-5.207166370D-06
 4.927572740D-09-1.709526276D-12                 -6.824035050D+03-7.757833983D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10324.814
 6.043066330D+05-2.646500381D+03 8.612474210D+00-5.532268240D-04 1.086845232D-07
-1.137381290D-11 4.904295520D-16                  4.845795180D+03-2.588861801D+01
DO2                Gurvich,1989 pt1 p138 pt2 p49.
 2 tpis89 D   1.00O   2.00    0.00    0.00    0.00 0   34.0129020       6487.344
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10065.344
-2.111479735D+04 6.023371750D+02-1.294877674D+00 1.812947970D-02-2.161807666D-05
 1.391729127D-08-3.697740280D-12                 -2.976943856D+03 3.272834480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10065.344
-1.267224927D+06 2.799947016D+03 2.325174609D+00 2.726325070D-03-6.314507320D-07
 6.729289200D-11-2.765192818D-15                 -1.959411733D+04 1.789922833D+01
DO2-               Gurvich,1989 pt1 p139 pt2 p50.
 2 tpis89 D   1.00O   2.00E   1.00    0.00    0.00 0   34.0134506      -104795.510
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10079.890
 1.048705051D+05-8.906236770D+02 5.666553560D+00 1.904603784D-03-1.215263210D-06
 6.577513330D-10-2.147376147D-13                 -8.942377250D+03-7.797219200D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10079.890
 5.527661920D+05-2.796895783D+03 8.772206670D+00-6.291116630D-04 1.272331622D-07
-1.364440687D-11 6.005199440D-16                  2.512066767D+03-2.890020381D+01
D2                 Ref-Species. Gurvich,1989 pt1 p134 pt2 p45.
 3 tpis89 D   2.00    0.00    0.00    0.00    0.00 0    4.0282040          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8569.103
 2.125790482D+04-2.996945907D+02 5.130314980D+00-4.172970890D-03 5.014345720D-06
-2.126389969D-09 2.386536969D-13                  3.944985900D+02-1.164191209D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8569.103
 8.215168560D+05-2.365623159D+03 5.342974510D+00 6.928145990D-05-8.523671020D-08
 2.456447415D-11-1.960597698D-15                  1.434214587D+04-1.712600356D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8569.103
 4.899848740D+08-3.112892916D+05 7.945961340D+01-8.425828740D-03 4.789458020D-07
-1.390917969D-11 1.637606941D-16                  2.460108052D+06-6.637009520D+02
D2+                Chase,1998 p1041.
 2 j 9/77 D   2.00E  -1.00    0.00    0.00    0.00 0    4.0276554       1498568.325
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8651.000
-9.640959090D+04 1.243052385D+03-2.557714366D+00 1.343064234D-02-1.285600289D-05
 6.463421670D-09-1.337616868D-12                  1.730966171D+05 3.356314920D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8651.000
 9.255951350D+05-4.505219940D+03 1.103203365D+01-4.706089030D-03 1.838068460D-06
-3.135924623D-10 1.857684975D-14                  2.058298890D+05-5.283912240D+01
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Appendix D (*continued*)

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D2-                Chase,1998 p1042.
 2 j 9/77 D   2.00E   1.00     0.00     0.00     0.00 0    4.0287526      235160.621
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8713.851
-4.365332060D+03 3.112987057D+02 5.481950030D-01 9.956988110D-03-1.167000612D-05
 6.975656410D-09-1.682718179D-12                  2.597897625D+04 1.442223161D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8713.851
-5.798805190D+04-3.122959355D+02 4.730388280D+00 5.695900800D-05 2.018975430D-08
-2.311492448D-12 1.070266527D-16                  2.851200896D+04-9.157527920D+00
D2O                Gurvich,1989 pt1 p142 pt2 p51.
 2 g 6/99 D   2.00O   1.00     0.00     0.00     0.00 0   20.0276040     -249210.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9960.017
 6.958278470D+03-1.280889437D+01 3.595878870D+00 1.502093683D-03 3.594675050D-07
 5.340417200D-10-5.181941270D-13                 -3.101944566D+04 2.895556576D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9960.017
 1.544193253D+06-5.474238900D+03 1.017542424D+01-9.619415540D-04 2.036545675D-07
-2.050566442D-11 8.510770690D-16                  2.983248980D+03-4.465011570D+01
D2O2               Gurvich,1989 pt1 p142 pt2 p52.
 2 g 6/99 D   2.00O   2.00     0.00     0.00     0.00 0   36.0270040     -144300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11565.639
 2.957711324D+04-6.893037570D+01 2.043905473D+00 1.570281822D-02-1.935478714D-05
 1.384941336D-08-4.104184900D-12                 -1.802502679D+04 1.347156482D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11565.639
 1.147867936D+06-5.225760930D+03 1.311088701D+01-1.179811896D-03 2.729336904D-07
-2.961433535D-11 1.310306129D-15                  1.219580532D+04-5.690538200D+01
D2S                Miller,1967. H2S data.
 2 g 6/01 D   2.00S   1.00     0.00     0.00     0.00 0   36.0932040     -24006.550
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10088.553
 3.988386480D+03-6.620792560D+01 4.393354450D+00-2.325113084D-03 1.189503465D-05
-1.146524521D-08 3.626190450D-12                 -3.787385550D+03 9.238754375D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10088.553
 4.235814630D+05-2.823776231D+03 8.962821840D+00-6.469231230D-04 1.634615644D-07
-1.797991376D-11 8.160939570D-16                  1.204603509D+04-3.191047376D+01
F                  Hf:Cox,1989.  Moore,1971. Moore,1970a. Gordon,1999.
 3 g 5/97 F   1.00     0.00     0.00     0.00     0.00 0   18.9984032      79380.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6518.460
 1.137409088D+03-1.453392797D+02 4.077403610D+00-4.303360140D-03 5.728897740D-06
-3.819312900D-09 1.018322509D-12                  9.311110120D+03-3.558982650D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6518.460
 1.473506226D+04 8.149927360D+01 2.444371819D+00 2.120210026D-05-4.546918620D-09
 5.109528730D-13-2.333894647D-17                  8.388374650D+03 5.478710640D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6518.460
-2.926724756D+07 1.775674924D+04-1.814463258D+00 5.351200280D-04-3.513620800D-08
 1.101519690D-12-1.061293837D-17                 -1.319642721D+05 4.248814560D+01
F+                 Moore,1971. Moore,1970a. Gordon,1999.
 3 g 3/97 F   1.00E  -1.00     0.00     0.00     0.00 0   18.9978546    1766816.332
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6710.732
-3.871680190D+04 3.218815660D+02 2.200920452D+00-2.455492688D-04 7.858355060D-07
-6.435987920D-10 1.839793564D-13                  2.098830937D+05 7.816999240D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6710.732
 1.649635664D+04 1.337351478D+02 2.332522942D+00 1.215277877D-04-4.801037700D-08
 9.027225150D-12-5.470664940D-16                  2.110745327D+05 6.625817090D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6710.732
 7.599619330D+06-1.391106563D+03 1.714871534D+00 2.428311844D-04-1.894860146D-08
 6.420828070D-13-8.257979730D-18                  2.269126001D+05 1.102848944D+01
F-                 Hotop,1985. Gordon,1999.
 3 g 1/98 F   1.00E   1.00     0.00     0.00     0.00 0   18.9989518     -255092.072
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.142572443D+04 3.264882710D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.142572443D+04 3.264882710D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.142572443D+04 3.264882710D+00
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FCN                Gurvich,1991 pt1 p229 pt2 p217.
 2 g 5/99 F   1.00C   1.00N   1.00    0.00    0.00 0   45.0158032      34327.854
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10128.960
 3.984454120D+04-6.988655360D+02 7.058839660D+00-1.404863382D-03 3.964652510D-06
-3.045609294D-09 7.923045900D-13                 6.172627570D+03-1.505643174D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10128.960
 3.981873550D+05-2.302971079D+03 9.027081390D+00-5.228710260D-04 1.191059272D-07
-1.280287231D-11 5.733807190D-16                 1.588449451D+04-2.984971982D+01
FCO                Hf:Gurvich,1991 pt1 p87. Jacox,1998 p193.
 2 g12/99 F   1.00C   1.00O   1.00    0.00    0.00 0   47.0085032    -179418.150
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10387.955
 1.132662744D+04-5.397918500D+01 2.966927601D+00 7.559959350D-03-6.211773580D-06
 2.403781550D-09-3.369507750D-13                -2.240369579D+04 1.092652142D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10387.955
-6.085851580D+04-1.022397533D+03 7.527322560D+00-1.057942328D-04-1.365311093D-09
 2.484612871D-12-9.997916800D-17                -1.805098416D+04-1.630331278D+01
FO                 Chase,1996b p582.
 2 j 9/95 F   1.00O   1.00    0.00    0.00    0.00 0   34.9978032     109012.100
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9388.000
-3.912182440D+04 7.967036940D+02-1.634777767D+00 1.601810071D-02-2.095210771D-05
 1.382740666D-08-3.664524950D-12                 8.375525230D+03 3.383325720D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9388.000
-1.597940503D+06 4.377376380D+03-4.897507640D-01 2.682336321D-03-6.900804850D-07
 7.246479680D-11-2.726912632D-15                -1.644248211D+04 3.559923610D+01
FO2,FOO            Chase,1996b p582.
 2 j 9/95 F   1.00O   2.00    0.00    0.00    0.00 0   50.9972032      25400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11255.812
 5.821564000D+03-2.347363967D+02 5.437338760D+00 2.165855252D-03 3.671472190D-07
-2.071530827D-09 9.431066850D-13                 2.694856027D+03-1.168202057D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11255.812
-1.213166895D+06 2.493397189D+03 4.465065740D+00 9.416104040D-04-6.426472260D-08
-1.085643277D-11 1.216995394D-15                -1.596800286D+04 8.655193180D+00
FO2,OFO            Chase,1996b p583.
 2 j 9/95 F   1.00O   2.00    0.00    0.00    0.00 0   50.9972032     378600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10538.382
-7.734106400D+04 1.663800209D+03-9.612815160D+00 4.989156870D-02-6.946217130D-05
 4.707787800D-08-1.258890729D-11                 3.697092730D+04 7.795943040D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10538.382
-6.211867340D+05 9.369474590D+02 6.401558750D+00 2.136110846D-04-4.337977650D-08
 4.667312240D-12-2.059767432D-16                 3.638357270D+04-6.150264330D+00
F2                 Ref-Elm. Gurvich,1989. pt1 p157 pt2 p73.
 2 tpis89 F   2.00    0.00    0.00    0.00    0.00 0   37.9968064          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8825.106
 1.018176308D+04 2.274241183D+01 1.971353040D+00 8.151604010D-03-1.148960090D-05
 7.958652530D-09-2.167079526D-12                -9.586943000D+02 1.130600296D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8825.106
-2.941167790D+06 9.456597700D+03-7.738616150D+00 7.644712990D-03-2.241007605D-06
 2.915845236D-10-1.425033974D-14                -6.071005610D+04 8.423835080D+01
F2O                Gurvich,1989 pt1 p161 pt2 p76.
 2 g 4/99 F   2.00O   1.00    0.00    0.00    0.00 0   53.9962064      24500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10911.521
 3.082919995D+04-2.299506259D+02 2.603805825D+00 1.586111264D-02-2.345633734D-05
 1.679619314D-08-4.703560330D-12                 3.055185332D+03 1.050933022D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10911.521
-1.885374518D+05-2.100729689D+02 7.151239160D+00 1.327687906D-04 1.804705706D-08
-1.416973671D-12 6.489389390D-17                 1.449129965D+03-1.257858336D+01
F2O2               FOOF. Chase,1996b p585.
 2 j 9/95 F   2.00O   2.00    0.00    0.00    0.00 0   69.9956064      19200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13778.453
 5.612270460D+04-9.985952230D+02 8.980649390D+00 6.421900870D-03-9.888516020D-06
 6.858061010D-09-1.842137493D-12                 5.298712590D+03-2.239292195D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13778.453
-2.190563532D+05-3.910920810D+02 1.029107144D+01-1.163345202D-04 2.570922521D-08
-2.949199983D-12 1.367386916D-16                 8.278020940D+02-2.756752555D+01
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FS2F              Difluorodisulfane. Chase,1998 p1146.
 2 j 6/76 F   2.00S   2.00     0.00     0.00     0.00 0  102.1268064     -336435.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14595.300
 1.144462280D+05-1.853247564D+03 1.394098518D+01-4.043689370D-03 1.370970316D-06
 6.711903100D-10-4.624954960D-13                 -3.351068330D+04-4.849215357D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14595.300
-2.077097921D+05-1.094539831D+02 1.008136946D+01-3.239537910D-05 7.125225270D-09
-8.134787410D-13 3.755022410D-17                 -4.349446060D+04-2.346916058D+01
Fe                Hf:Hultgren,1973. Sugar,1985. Gordon,1999.
 3 g 5/97 FE  1.00    0.00     0.00     0.00     0.00 0   55.8450000      415471.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6850.327
 6.790822660D+04-1.197218407D+03 9.843393310D+00-1.652324828D-02 1.917939959D-05
-1.149825371D-08 2.832773807D-12                  5.466995940D+04-3.383946260D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6850.327
-1.954923682D+06 6.737161100D+03-5.486410970D+00 4.378803450D-03-1.116286672D-06
 1.544348856D-10-8.023578182D-15                  7.137370060D+03 6.504979860D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6850.327
 1.216352511D+09-5.828563930D+05 9.789634510D+01-5.370704430D-03 3.192037920D-08
 6.267671430D-12-1.480574914D-16                  4.847648290D+06-8.697289770D+02
Fe+               Sugar,1985. Gordon,1999.
 3 g 3/98 FE  1.00E  -1.00     0.00     0.00     0.00 0   55.8444514     1184217.849
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6935.749
-5.691231620D+04 1.847134390D+02 4.196972120D+00-5.978275970D-03 1.054267912D-05
-8.059804320D-09 2.256925874D-12                  1.401206571D+05-3.602542580D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6935.749
-8.176450090D+05 1.925359408D+03 1.717387154D+00 3.385338980D-04-9.813533120D-08
 2.228179208D-11-1.483964439D-15                  1.286352466D+05 1.500256262D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6935.749
 1.065217491D+08-2.883923997D+04-2.821752459D+00 2.712846797D-03-3.107069182D-07
 1.543726493D-11-2.725133516D-16                  4.142981690D+05 4.053497330D+01
Fe-                Hotop,1985. Gordon,1999.
 3 g 9/97 FE  1.00E   1.00     0.00     0.00     0.00 0   55.8455486      393338.036
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6641.836
 1.341276767D+05-1.775438064D+03 1.084366935D+01-1.499440282D-02 1.412129744D-05
-6.942189050D-09 1.410953082D-12                  5.519472530D+04-4.140886490D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6641.836
-1.237808631D+05 8.249279070D+02 1.912936452D+00 2.280194065D-04-4.942014160D-08
 5.591493490D-12-2.566386941D-16                  4.156251610D+04 1.265367627D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6641.836
-1.008467687D+06 7.642402360D+02 2.332880311D+00 1.892649914D-05-1.170322571D-09
 3.749758920D-14-4.871021520D-19                  4.111417150D+04 9.680921840D+00
Fe(CO)5           Chase,1998 p698.
 2 j 3/78 FE  1.00C   5.00O   5.00     0.00     0.00 0  195.8955000     -727850.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33145.399
 3.797805710D+05-7.285928160D+03 5.400236180D+01-6.935400750D-02 1.026705717D-04
-7.207373130D-08 1.958981996D-11                 -5.854580480D+04-2.604377836D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33145.399
 1.116600852D+06-8.067074730D+03 3.652942410D+01-2.047190300D-03 4.441967750D-07
-4.932507130D-11 2.235704865D-15                 -4.860661250D+04-1.754566113D+02
FeCL              Chase,1998 p761.
 2 j 6/65 FE  1.00CL  1.00     0.00     0.00     0.00 0   91.2980000      251040.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10377.153
 1.117340353D+04-5.402144290D+01 3.486057920D+00 6.879837140D-03-1.273679557D-05
 1.025321859D-08-3.051544011D-12                  2.928681990D+04 9.428962979D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10377.153
 5.288700220D+05-1.282897413D+03 5.798441690D+00-2.896589776D-04 3.343903810D-08
-1.469606582D-13-1.213444602D-16                  3.726196730D+04-4.075134191D+00
FeCL2             Chase,1998 p822.
 2 j12/70 FE  1.00CL  2.00     0.00     0.00     0.00 0  126.7510000     -141000.800
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14277.338
 2.301121607D+04-5.858044060D+02 9.322903480D+00-3.006298824D-03 2.590788666D-06
-1.080178662D-09 2.341239608D-13                 -1.621041276D+04-1.816752393D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14277.338
 1.644123697D+05 6.928002690D+02 4.638270140D+00 2.754339782D-03-8.624218250D-07
 1.170827576D-10-5.938061950D-15                 -2.219721855D+04 1.116897701D+01
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FeCL3             Chase,1998 p879.
 2 j 6/65 FE  1.00CL  3.00    0.00    0.00    0.00 0  162.2040000   -1059104.288
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18214.073
 4.284772100D+03-5.741705370D+02 1.220667256D+01-4.680434120D-03 5.609500470D-06
-3.549599500D-09 9.198543490D-13                -1.275688456D+05-2.887584081D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18214.073
-5.915740590D+04-1.033382228D+01 1.000849967D+01-3.657651870D-06 8.545873640D-10
-1.023070527D-13 4.904063640D-18                -1.305012050D+05-1.598494171D+01
FeO               Chase,1998 p1239.
 2 j 9/66 FE  1.00O   1.00    0.00    0.00    0.00 0   71.8444000     251040.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8837.031
 1.569282213D+04-6.460188880D+01 2.458925470D+00 7.016047360D-03-1.021405947D-05
 7.179297870D-09-1.978966365D-12                 2.964572665D+04 1.326115545D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8837.031
-1.195971480D+05-3.624864780D+02 5.518880750D+00-9.978856890D-04 4.376913830D-07
-6.790629460D-11 3.639292680D-15                 3.037985806D+04-3.633655420D+00
Fe(OH)2           Chase,1998 p1230.
 2 j12/66 FE  1.00O   2.00H   2.00    0.00    0.00 0   89.8596800    -330536.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14209.461
 4.443027200D+05-6.795140890D+03 3.894726210D+01-5.973005680D-02 7.046165430D-05
-4.087859510D-08 9.368766340D-12                -9.051420860D+03-1.931304058D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14209.461
 1.612519190D+06-6.533241990D+03 1.842922816D+01-2.073249635D-03 4.265874360D-07
-4.564063130D-11 1.990105746D-15                -2.992568633D+03-8.445940590D+01
Fe2CL4            Chase,1998 p891.
 2 j12/70 FE  2.00CL  4.00    0.00    0.00    0.00 0  253.5020000    -431370.400
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29849.201
 1.501308814D+03-6.617096510D+02 1.826924882D+01-4.181494660D-03 4.196535050D-06
-2.188670747D-09 5.395194700D-13                -5.340057580D+04-4.935640680D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29849.201
 1.402450973D+05 6.936064410D+02 1.313800410D+01 2.754333070D-03-8.623996010D-07
 1.170782491D-10-5.937778080D-15                -5.974172730D+04-1.752491511D+01
Fe2CL6            Chase,1998 p928.
 2 j 6/65 FE  2.00CL  6.00    0.00    0.00    0.00 0  324.4080000    -654377.600
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         40447.854
-1.034544447D+04-8.234876600D+02 2.520090594D+01-6.845796790D-03 8.255820750D-06
-5.248965660D-09 1.365242237D-12                -8.131847190D+04-8.010768938D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         40447.854
-9.999118000D+04-1.457716085D+01 2.201208460D+01-5.229481130D-06 1.226831608D-09
-1.473195806D-13 7.078272330D-18                -8.551496190D+04-6.143757198D+01
Ga                Hf:Gurvich,1996a. Moore,1971. Johansson,1966. Gordon,1999.
 3 g12/98 GA  1.00    0.00    0.00    0.00    0.00 0   69.7230000     272000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6551.115
 2.387947890D+05-3.121634631D+03 1.630171272D+01-2.347922342D-02 1.932327565D-05
-7.316311870D-09 8.857387735D-13                 4.732717380D+04-7.547172760D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6551.115
-5.544186520D+04 8.808624420D+02 1.760717716D+00 2.993259460D-04-5.610827310D-08
 2.682832239D-12 3.132134914D-16                 2.684351822D+04 1.252212023D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6551.115
 2.288759836D+08-6.759297920D+04 2.526821493D+00 1.463058875D-03-1.250892936D-07
 3.820116110D-12-3.997883065D-17                 6.402915740D+05-8.083504020D+00
Ga+               IP:Johansson,1966. Moore,1971. Gordon,1999.
 3 g12/98 GA  1.00E  -1.00    0.00    0.00    0.00 0   69.7224514     856688.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21                 1.022899726D+05 5.215090460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 3.566607140D+04-1.108845546D+02 2.635517951D+00-8.338973520D-05 2.734243614D-08
-4.555673740D-12 3.035050101D-16                 1.029897430D+05 4.257075410D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.880791061D+08-1.410890480D+05 4.500268850D+01-6.445582900D-03 5.005999840D-07
-1.789454995D-11 2.439723414D-16                 1.191428220D+06-3.545671850D+02
GaBr              Gurvich,1996a pt1 p239 pt2 p193
 2 tpis96 GA  1.00BR  1.00    0.00    0.00    0.00 0  149.6270000    -17967.880
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9932.119
-2.185275415D+03-7.672232970D+01 4.770805670D+00-4.497881060D-04 5.579853600D-07
-3.065156457D-10 7.042946040D-14                -3.138004818D+03 2.948144294D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9932.119
 3.359805030D+05-8.406836680D+02 5.145084730D+00-3.265526000D-05-7.671022750D-08
 3.635123820D-11-3.358177830D-15                 2.035179445D+03-4.277894080D-01
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GaBr2              Gurvich,1996a pt1 p241 pt2 p194.
 2 tpis96 GA  1.00BR  2.00     0.00     0.00     0.00 0  229.5310000     -149180.952
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14024.948
 7.081681620D+03-3.705766100D+02 8.418425360D+00-3.001930915D-03 3.595477670D-06
-2.276883735D-09 5.913221770D-13                -1.821116655D+04-9.512572050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14024.948
-3.302294360D+05 4.766722650D+02 7.104725400D+00-5.522771210D-04 3.159876015D-07
-5.513637150D-11 3.173293230D-15                -2.365683620D+04-1.162714892D+00
GaBr3              Gurvich,1996a pt1 p243 pt2 p196.
 2 tpis96 GA  1.00BR  3.00     0.00     0.00     0.00 0  309.4350000     -292962.663
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19037.337
 6.363807340D+03-5.142040450D+02 1.196065138D+01-4.134637650D-03 4.933978330D-06
-3.111868526D-09 8.043631480D-13                -3.570415500D+04-2.556896053D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19037.337
-5.103063750D+04-9.395209690D+00 1.000768765D+01-3.295954300D-06 7.679838140D-10
-9.175147260D-14 4.391186940D-18                -3.833402150D+04-1.410315914D+01
GaCL               Gurvich,1996a pt1 p231 pt2 p186
 2 tpis96 GA  1.00CL  1.00     0.00     0.00     0.00 0  105.1760000      -69621.440
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9609.116
 6.417143000D+03-2.257949147D+02 5.311673690D+00-1.562280975D-03 1.836579731D-06
-1.100421873D-09 2.725812445D-13                -8.593892330D+03-1.695911735D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9609.116
-4.864842240D+05 1.452870183D+03 2.719542959D+00 1.144285628D-03-3.431452860D-07
 5.470440480D-11-3.019622103D-15                -1.895084035D+04 1.570926145D+01
GaCL2              Gurvich,1996a pt1 p232 pt2 p187.
 2 tpis96 GA  1.00CL  2.00     0.00     0.00     0.00 0  140.6290000     -220978.909
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13513.391
 2.225481851D+04-6.046218440D+02 9.220388910D+00-4.554400790D-03 5.324855180D-06
-3.308605570D-09 8.462235560D-13                -2.564550386D+04-1.685409262D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13513.391
-3.445405300D+05 4.714437160D+02 7.108775480D+00-5.539433560D-04 3.163638240D-07
-5.518023930D-11 3.175353030D-15                -3.230936160D+04-3.744840740D+00
GaCL3              Gurvich,1996a pt1 p235 pt2 p189.
 2 tpis96 GA  1.00CL  3.00     0.00     0.00     0.00 0  176.0820000     -432624.753
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17375.247
 4.784948400D+04-1.162678125D+03 1.408954213D+01-8.106134290D-03 9.219430160D-06
-5.599710550D-09 1.404852600D-12                -4.915909730D+04-4.282179383D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17375.247
-9.466917310D+04-2.561468254D+01 1.002010048D+01-8.354073070D-06 1.901439055D-09
-2.231168493D-13 1.052949609D-17                -5.518201430D+04-1.864958383D+01
GaF                Gurvich,1996a pt1 p224 pt2 p179
 2 tpis96 GA  1.00F   1.00     0.00     0.00     0.00 0   88.7214032     -232608.491
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9081.109
 3.670398010D+04-5.336572220D+02 5.759291920D+00-1.506128492D-03 9.509038450D-07
-1.830941130D-10-3.135959193D-14                -2.647075690D+04-6.589321880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9081.109
-2.983392279D+05 7.225157870D+02 3.639557430D+00 5.546736760D-04-1.464901450D-07
 2.177385396D-11-1.031058874D-15                -3.408528710D+04 7.553960000D+00
GaF2               Gurvich,1996a pt1 p225 pt2 p180.
 2 tpis96 GA  1.00F   2.00     0.00     0.00     0.00 0  107.7198064     -516712.441
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12115.659
 6.842539530D+04-8.897617740D+02 7.707455490D+00 2.072150890D-03-5.289981930D-06
 4.564127420D-09-1.406942753D-12                -5.919856150D+04-1.341142116D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12115.659
 4.100251360D+05-1.723259472D+03 8.951329220D+00-1.059205682D-03 2.745755154D-07
-2.907681311D-11 1.084834142D-15                -5.376571600D+04-2.113835528D+01
GaF3               Gurvich,1996a pt1 p226 pt2 p182.
 2 tpis96 GA  1.00F   3.00     0.00     0.00     0.00 0  126.7182096     -921476.983
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15223.017
 9.593266700D+04-1.355507494D+03 1.097760197D+01 3.461571720D-03-8.469551950D-06
 7.222468930D-09-2.213328653D-12                -1.061479087D+05-3.212651850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15223.017
-2.096961760D+05-1.431211274D+02 1.010568378D+01-4.184936820D-05 9.164759450D-09
-1.042661957D-12 4.799163450D-17                -1.136678134D+05-2.392539330D+01
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GaH               Gurvich,1996a pt1 p220 pt2 p177
 2 tpis96 GA  1.00H   1.00     0.00     0.00     0.00 0   70.7309400      214323.404
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8673.104
-4.391876200D+04 6.254457120D+02 3.276862890D-01 6.496641500D-03-3.802970010D-06
 2.852103704D-10 3.626809130D-13                  2.171260108D+04 2.224032244D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8673.104
 3.257993990D+06-1.109099502D+04 1.801126796D+01-8.167719110D-03 2.601293566D-06
-3.813459350D-10 2.028049649D-14                  9.369778240D+04-9.820900220D+01
GaI               Gurvich,1996a pt1 p247 pt2 p200
 2 tpis96 GA  1.00I   1.00     0.00     0.00     0.00 0  196.6274700      44871.122
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10109.122
-3.661855030D+03-3.206924180D+01 4.599961920D+00-8.899475460D-05 1.162792633D-07
-1.812351457D-11-7.584619640D-15                  4.198649370D+03 4.928964650D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10109.122
 1.498356654D+06-4.551967240D+03 9.803005350D+00-2.943735609D-03 8.658040510D-07
-1.106638204D-10 5.007836860D-15                  3.291811910D+04-3.227359770D+01
GaI2              Gurvich,1996a pt1 p249 pt2 p201.
 2 tpis96 GA  1.00I   2.00     0.00     0.00     0.00 0  323.5319400     -28954.965
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14470.935
-9.831395900D+02-2.152621259D+02 7.844318760D+00-1.819797849D-03 2.210706958D-06
-1.416110855D-09 3.713762930D-13                 -4.534090230D+03-4.250516810D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14470.935
-3.202879750D+05 4.796502330D+02 7.102333960D+00-5.512657830D-04 3.157543452D-07
-5.510871940D-11 3.171977730D-15                 -9.180919610D+03 7.275204880D-01
GaI3              Gurvich,1996a pt1 p250 pt2 p203.
 2 tpis96 GA  1.00I   3.00     0.00     0.00     0.00 0  450.4364100    -115877.240
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20122.760
-5.663472650D+03-2.425937116D+02 1.095451119D+01-2.059175489D-03 2.499117622D-06
-1.596502506D-09 4.167644060D-13                 -1.576722832D+04-1.646129942D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20122.760
-3.164040130D+04-4.208662830D+00 1.000352001D+01-1.532650180D-06 3.611531540D-10
-4.350978870D-14 2.095704875D-18                 -1.700058453D+04-1.090291552D+01
GaO               Gurvich,1996a pt1 p214 pt2 p174
 2 tpis96 GA  1.00O   1.00     0.00     0.00     0.00 0   85.7224000      146823.607
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8925.107
 7.325543910D+04-9.804269510D+02 7.844122760D+00-7.171072850D-03 7.872780510D-06
-2.401464112D-09-2.594919458D-13                  2.140581724D+04-1.799742951D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8925.107
 2.937313804D+06-1.118314112D+04 1.859366773D+01-6.854753450D-03 1.665399251D-06
-1.887560878D-10 7.972686920D-15                  8.530248080D+04-9.904040480D+01
GaOH              Gurvich,1996a pt1 p222 pt2 p178.
 2 tpis96 GA  1.00O   1.00H    1.00     0.00     0.00 0   86.7303400     -143630.495
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10583.608
 6.963101870D+04-1.247828695D+03 1.022001611D+01-5.922534390D-03 4.643387400D-06
-1.215936978D-09-2.945243614D-14                 -1.275397794D+04-3.217063000D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10583.608
 8.429051010D+05-2.372324595D+03 8.009071090D+00 8.777230710D-05-5.943068910D-08
 9.841943440D-12-5.531552790D-16                 -3.751788250D+03-2.171053719D+01
Ga2Br2            Gurvich,1996a pt1 p244 pt2 p197.
 2 tpis96 GA  2.00BR  2.00     0.00     0.00     0.00 0  299.2540000     -136963.692
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20793.308
-1.117183241D+04-7.471471620D+01 1.030246084D+01-6.657929850D-04 8.200515850D-07
-5.297021520D-10 1.394553192D-13                 -1.913297856D+04-1.317110316D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20793.308
-1.885373131D+04-1.263621802D+00 1.000108034D+01-4.774975660D-07 1.137227648D-10
-1.380820486D-14 6.690242430D-19                 -1.951053843D+04-1.141667594D+01
Ga2Br4            Gurvich,1996a pt1 p245 pt2 p198.
 2 tpis96 GA  2.00BR  4.00     0.00     0.00     0.00 0  459.0620000     -415820.034
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         30591.766
-1.315545939D+04-4.136553020D+02 1.762849229D+01-3.514652160D-03 4.266937730D-06
-2.726515882D-09 7.118924490D-13                 -5.283101810D+04-4.427520690D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         30591.766
-5.742167210D+04-7.160137370D+00 1.600598947D+01-2.608182270D-06 6.146455950D-10
-7.405438650D-14 3.567126630D-18                 -5.493389760D+04-3.479271660D+01
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Ga2Br6            Gurvich,1996a pt1 p246 pt2 p199.
 2 tpis96 GA  2.00BR  6.00    0.00    0.00    0.00 0  618.8700000    -673688.732
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         41151.266
-6.725116890D+03-8.067526550D+02 2.511671424D+01-6.636514570D-03 7.977555700D-06
-5.059685210D-09 1.313546388D-12                -8.370635200D+04-7.585278720D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         41151.266
-9.526173000D+04-1.444681880D+01 2.201192546D+01-5.145006740D-06 1.204348449D-09
-1.443806473D-13 6.928270740D-18                -8.782223300D+04-5.765895120D+01
Ga2CL2            Gurvich,1996a pt1 p237 pt2 p190.
 2 tpis96 GA  2.00CL  2.00    0.00    0.00    0.00 0  210.3520000    -220972.686
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19488.425
-9.246133700D+03-2.592159934D+02 1.102847129D+01-2.231983927D-03 2.720723456D-06
-1.743798624D-09 4.563666040D-13                -2.834059821D+04-2.067773272D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19488.425
-3.668954200D+04-4.434580680D+00 1.000373051D+01-1.630793333D-06 3.853753320D-10
-4.652527730D-14 2.244498791D-18                -2.965633085D+04-1.469535817D+01
Ga2CL4            Gurvich,1996a pt1 p237 pt2 p191.
 2 tpis96 GA  2.00CL  4.00    0.00    0.00    0.00 0  281.2580000    -602326.828
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27315.392
 1.637343702D+04-1.140637354D+03 2.030139827D+01-8.997746200D-03 1.067254867D-05
-6.700290620D-09 1.725749144D-12                -7.162385010D+04-6.666361900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27315.392
-1.127110409D+05-2.138517542D+01 1.601738077D+01-7.415564640D-06 1.721694751D-09
-2.051361953D-13 9.797311500D-18                -7.746853380D+04-4.147280870D+01
Ga2CL6            Gurvich,1996a pt1 p238 pt2 p192.
 2 tpis96 GA  2.00CL  6.00    0.00    0.00    0.00 0  352.1640000    -962463.532
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         36359.799
 6.089469840D+04-2.104456302D+03 2.959653878D+01-1.537809796D-02 1.779096808D-05
-1.095619429D-08 2.779706493D-12                -1.118400535D+05-1.121945814D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         36359.799
-1.898445426D+05-4.413655240D+01 2.203505047D+01-1.470071128D-05 3.369512810D-09
-3.975462800D-13 1.884231868D-17                -1.226969998D+05-6.745332883D+01
Ga2F2             Gurvich,1996a pt1 p228 pt2 p183.
 2 tpis96 GA  2.00F   2.00    0.00    0.00    0.00 0  177.4428064    -606231.344
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17147.856
 2.978130650D+04-1.013975520D+03 1.374933053D+01-7.728050960D-03 9.064007330D-06
-5.641193220D-09 1.443106716D-12                -7.086083370D+04-4.109833950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17147.856
-8.773234930D+04-1.983775870D+01 1.001594030D+01-6.744402830D-06 1.556129063D-09
-1.845316975D-13 8.780884020D-18                -7.607368630D+04-1.908325521D+01
Ga2F4             Gurvich,1996a pt1 p228 pt2 p184.
 2 tpis96 GA  2.00F   4.00    0.00    0.00    0.00 0  215.4396128   -1325002.958
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22653.242
 1.422079998D+05-2.798829941D+03 2.395904235D+01-1.293904774D-02 1.223101326D-05
-6.251209820D-09 1.334919195D-12                -1.496013710D+05-9.734153640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22653.242
-2.704366090D+05-1.049957196D+02 1.607903965D+01-3.178895920D-05 7.049582720D-09
-8.102379520D-13 3.760540530D-17                -1.644169589D+05-4.896591730D+01
Ga2F6             Gurvich,1996a pt1 p230 pt2 p185.
 2 tpis96 GA  2.00F   6.00    0.00    0.00    0.00 0  253.4364192   -2017623.843
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         30131.476
 2.409045572D+05-4.142379800D+03 3.195773720D+01-1.297914290D-02 8.959282190D-06
-2.733621068D-09 1.554030994D-13                -2.272785240D+05-1.398403732D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         30131.476
-4.368664800D+05-2.128208368D+02 2.215886373D+01-6.346287910D-05 1.399738556D-08
-1.601732039D-12 7.407584420D-17                -2.494298707D+05-7.787635830D+01
Ga2I2             Gurvich,1996a pt1 p252 pt2 p204.
 2 tpis96 GA  2.00I   2.00    0.00    0.00    0.00 0  393.2549400    13520.947
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21497.947
-8.960252670D+03-3.172057210D+01 1.012930491D+01-2.860191165D-04 3.535333010D-07
-2.289632389D-10 6.040085360D-14                -1.233174068D+03-9.801968380D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21497.947
-1.219056501D+04-5.287554470D-01 1.000045392D+01-2.011599344D-07 4.799467810D-11
-5.834781080D-15 2.829565069D-19                -1.393258606D+03-9.052614910D+00
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Ga2I4              Gurvich,1996a pt1 p253 pt2 p205.
 2 tpis96 GA  2.00I   4.00     0.00     0.00     0.00 0  647.0638800     -159267.987
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          32583.813
-1.769495991D+04-1.354871509D+02 1.654625333D+01-1.199014713D-03 1.473754848D-06
-9.504796570D-10 2.499380837D-13                 -2.333405795D+04-3.325712890D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          32583.813
-3.171299760D+04-2.287068836D+00 1.600194812D+01-8.588964380D-07 2.041966602D-10
-2.476145769D-14 1.198551944D-18                 -2.401940505D+04-3.008672521D+01
Ga2I6              Gurvich,1996a pt1 p253 pt2 p206.
 2 tpis96 GA  2.00I   6.00     0.00     0.00     0.00 0  900.8728200     -317294.623
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          43573.378
-2.110891458D+04-3.695404160D+02 2.346811836D+01-3.189178210D-03 3.890339040D-06
-2.494830378D-09 6.532007280D-13                 -4.301188090D+04-6.014811500D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          43573.378
-6.015698150D+04-6.329209230D+00 2.200533040D+01-2.332008629D-06 5.513868480D-10
-6.659445350D-14 3.213670430D-18                 -4.488699380D+04-5.161008750D+01
Ga2O               Gurvich,1996a pt1 p216 pt2 p175.
 2 tpis96 GA  2.00O   1.00     0.00     0.00     0.00 0  155.4454000      -99457.457
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12162.595
 5.697197180D+04-8.074085990D+02 7.733061540D+00 1.478450874D-03-4.097743430D-06
 3.581158920D-09-1.107073202D-12                 -9.512216820D+03-1.256149299D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12162.595
-1.193874986D+05-8.719341610D+01 7.064678200D+00-2.571524542D-05 5.651108490D-09
-6.448190540D-13 2.975374645D-17                 -1.393694796D+04-6.942801300D+00
Ge                 Hf:Gurvich,1991 pt1 p311. Sugar,1993. Gordon,1999.
 3 g 3/99 GE  1.00     0.00     0.00     0.00     0.00 0   72.6400000     367800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7398.584
-2.059215242D+04-1.432022103D+02 4.506002330D+00 1.547187840D-03-8.518296550D-06
 8.243824460D-09-2.566167305D-12                 4.363070860D+04-6.224648889D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7398.584
-8.565413840D+05 3.917958660D+03-1.809888212D+00 2.276482224D-03-5.365627550D-07
 5.984958090D-11-2.541700646D-15                 1.956518798D+04 3.841408752D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7398.584
 2.423965136D+07-2.543605174D+04 1.456087539D+01-2.592562254D-03 2.658628502D-07
-1.122785077D-11 1.620997559D-16                 2.295812461D+05-8.953523898D+01
Ge+                Sugar,1993. Gordon,1999.
 3 g 3/99 GE  1.00E  -1.00     0.00     0.00     0.00 0   72.6394514    1134984.385
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6205.785
-3.453666430D+05 4.008449710D+03-1.522395737D+01 3.626030020D-02-3.351367260D-05
 1.431059219D-08-2.236976459D-12                 1.157058042D+05 1.090158182D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6205.785
-2.244860570D+06 5.165531140D+03-3.867516510D-01 8.528730940D-04-1.386040003D-07
 1.155945775D-11-3.784413134D-16                 1.006823985D+05 2.965845411D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6205.785
 5.768056240D+07-3.078606210D+04 8.706291820D+00-4.942233500D-04-2.690467703D-11
 1.853441677D-12-5.082067525D-17                 3.857785420D+05-4.842537137D+01
Ge-                Hotop,1985. Gordon,1999.
 3 g 3/99 GE  1.00E   1.00     0.00     0.00     0.00 0   72.6405486     245402.540
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6980.940
 2.989142308D+03 8.657417230D+01 2.191868507D+00 5.900795270D-04-6.375800580D-07
 3.661132150D-10-8.689778450D-14                 2.835695190D+04 9.417623637D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6980.940
 1.352040246D+04-5.048518780D-01 2.500140247D+00-3.652944160D-09-6.716722200D-12
 1.378119925D-15-8.475212940D-20                 2.881739757D+04 7.577953867D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6980.940
 1.079877187D+04 1.149969180D+00 2.499738027D+00 3.051383052D-08-1.930296476D-12
 6.305166240D-17-8.327676240D-22                 2.880429709D+04 7.581467327D+00
GeBr               Gurvich,1991 pt1 p333 pt2 p287.
 2 tpis91 GE  1.00BR  1.00     0.00     0.00     0.00 0  152.5440000     137438.119
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9864.119
-5.680774630D+04 9.173361260D+02-2.224809366D+00 2.171239242D-02-3.035490868D-05
 2.011776305D-08-5.202915040D-12                 1.104192901D+04 4.107865983D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9864.119
 2.256750476D+05-7.310715460D+02 6.263283810D+00-1.198085447D-03 4.000377770D-07
-5.429937880D-11 2.510481953D-15                 1.942863606D+04-6.106507844D+00
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GeBr2              Gurvich,1991 pt1 p334 pt2 p288.
 2 tpis91 GE  1.00BR  2.00     0.00     0.00     0.00 0  232.4480000      -60962.897
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           14193.463
-1.649285325D+03-2.296262116D+02 7.900144680D+00-1.936685504D-03 2.345776175D-06
-1.496279368D-09 3.901453500D-13                 -8.316624210D+03-6.918156136D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           14193.463
-2.636655245D+04-3.990509020D+00 7.003327440D+00-1.445749787D-06 3.401591360D-10
-4.093457030D-14 1.969987842D-18                 -9.484999250D+03-1.673617098D+00
GeBr3              Gurvich,1991 pt1 p335 pt2 p289.
 2 tpis91 GE  1.00BR  3.00     0.00     0.00     0.00 0  312.3520000     -119031.308
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           18549.492
 2.725568677D+03-5.186213260D+02 1.199957754D+01-4.251024530D-03 5.103629720D-06
-3.233706250D-09 8.388358860D-13                 -1.477988251D+04-2.534555678D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           18549.492
-5.433926700D+04-9.280327950D+00 1.000765019D+01-3.297322150D-06 7.712929260D-10
-9.241571850D-14 4.432876230D-18                 -1.742697092D+04-1.366946296D+01
GeBr4              Gurvich,1991 pt1 p336 pt2 p290.
 2 tpis91 GE  1.00BR  4.00     0.00     0.00     0.00 0  392.2560000     -291000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           23963.218
 5.431940390D+03-6.777748800D+02 1.560015305D+01-5.507788880D-03 6.594764290D-06
-4.170146140D-09 1.080116643D-12                 -3.557606400D+04-4.209122927D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           23963.218
-6.977757910D+04-1.179873115D+01 1.300953955D+01-4.024938750D-06 9.203567210D-10
-1.076853369D-13 5.040954800D-18                 -3.904148160D+04-2.689436070D+01
GeCL               Gurvich,1991 pt1 p328 pt2 p283.
 2 tpis91 GE  1.00CL  1.00     0.00     0.00     0.00 0  108.0930000      69029.915
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9599.115
 1.069724739D+04-2.241238266D+01 1.987371070D+00 1.368270905D-02-2.358294414D-05
 1.786756020D-08-5.102503250D-12                  7.440683390D+03 1.505837189D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9599.115
-3.784193250D+05 1.429309204D+03 3.194854640D+00 8.119939120D-04-2.652459954D-07
 5.151957880D-11-3.534214570D-15                 -2.087046335D+03 1.385033820D+01
GeCL2              Gurvich,1991 pt1 p330 pt2 p284.
 2 tpis91 GE  1.00CL  2.00     0.00     0.00     0.00 0  143.5460000     -171000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13276.791
 1.838536673D+04-5.827205340D+02 9.161404660D+00-4.464786030D-03 5.244873550D-06
-3.268067210D-09 8.367575420D-13                 -1.975798598D+04-1.734321630D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13276.791
-4.890128920D+04-1.126210418D+01 7.009063530D+00-3.839180730D-06 8.865633570D-10
-1.052000540D-13 5.008422220D-18                 -2.275254424D+04-4.656641298D+00
GeCL3              Hf:Gurvich,1991 pt1 p331. Gurvich,1979 pt2 p287.
 2 g 6/01 GE  1.00CL  3.00     0.00     0.00     0.00 0  178.9990000     -266950.589
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           17559.437
 1.935859579D+04-8.342020000D+02 1.312702530D+01-6.511390020D-03 7.696277480D-06
-4.818541730D-09 1.238399959D-12                 -3.097218753D+04-3.552547184D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           17559.437
-7.574499820D+04-1.579213420D+01 1.001278835D+01-5.441738310D-06 1.260936724D-09
-1.500137106D-13 7.156400810D-18                 -3.525131720D+04-1.719719944D+01
GeCL4              Gurvich,1991 pt1 p332 pt2 p286.
 2 tpis91 GE  1.00CL  4.00     0.00     0.00     0.00 0  214.4520000     -500000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           21136.625
 6.502870410D+04-1.652482760D+03 1.881327000D+01-1.152426810D-02 1.310809980D-05
-7.961956110D-09 1.997505040D-12                 -5.570052390D+04-6.754438135D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           21136.625
-1.376261210D+05-3.603769500D+01 1.302816670D+01-1.164956960D-05 2.636193380D-09
-3.072926720D-13 1.439808750D-17                 -6.426281780D+04-3.318158305D+01
GeF                Gurvich,1991 pt1 p324 pt2 p279.
 2 tpis91 GE  1.00F   1.00     0.00     0.00     0.00 0   91.6384032      -70592.990
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9144.110
 5.017097820D+04-4.395552520D+02 2.990864513D+00 1.252766738D-02-2.337593226D-05
 1.841631179D-08-5.398492260D-12                 -7.093516400D+03 7.064248931D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9144.110
-5.150480580D+05 1.659711777D+03 2.999610299D+00 8.198511680D-04-2.271982948D-07
 3.624183860D-11-2.133840473D-15                 -2.051529487D+04 1.373154230D+01
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GeF2              Gurvich,1991 pt1 p326 pt2 p280.
 2 tpis91 GE  1.00F   2.00    0.00    0.00    0.00 0  110.6368064    -574000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11787.485
 7.543097080D+04-1.108456469D+03 9.078898270D+00-1.445630636D-03-6.575322320D-07
 1.475344103D-09-5.811220270D-13                -6.510685550D+04-2.200457134D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11787.485
-1.275327716D+05-7.162591350D+01 7.053002370D+00-2.101910441D-05 4.607893700D-09
-5.246394670D-13 2.416218951D-17                -7.112637630D+04-8.483841439D+00
GeF3              Hf:Gurvich,1991 pt1 p327. Gurvich,1979 v2 pt2 p283.
 2 g 6/01 GE  1.00F   3.00    0.00    0.00    0.00 0  129.6352096    -806332.833
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14678.187
 1.114121569D+05-1.776908030D+03 1.352166477D+01-2.983622949D-03-3.612749750D-08
 1.621528436D-09-7.199011780D-13                -9.038262960D+04-4.568760023D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14678.187
-2.069580129D+05-1.110233803D+02 1.008234122D+01-3.271676260D-05 7.183896700D-09
-8.190388120D-13 3.776322440D-17                -9.999749090D+04-2.303465940D+01
GeF4              Gurvich,1991 pt1 p328 pt2 p282.
 2 tpis91 GE  1.00F   4.00    0.00    0.00    0.00 0  148.6336128   -1190150.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17293.025
 1.119818968D+05-1.636859630D+03 1.231371005D+01 1.025446325D-02-1.893783072D-05
 1.476849261D-08-4.325174110D-12                -1.374265128D+05-4.104202391D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17293.025
-3.253032680D+05-2.538279448D+02 1.318792173D+01-7.460058550D-05 1.637384721D-08
-1.866482733D-12 8.605530500D-17                -1.466176526D+05-4.122237561D+01
GeH4              Barin,1989 pt1 p628.
 2 bar89  GE  1.00H   4.00    0.00    0.00    0.00 0   76.6717600       90793.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
-2.568398191D+05-4.132811450D+01 7.755116280D+00 2.129640783D-03 7.255053610D-07
-5.096314010D-10 1.431608261D-13                7.881538040D+03-2.030107999D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
-3.809805880D+06 1.093167093D+04-5.149675410D+00 9.485931370D-03-1.649459859D-06
 1.419674126D-10-5.004639750D-15                -6.158518520D+04 7.168961273D+01
GeI               Gurvich,1991 pt1 p337 pt2 p291.
 2 tpis91 GE  1.00I   1.00    0.00    0.00    0.00 0  199.5444700      210969.120
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10005.120
-7.438308220D+04 1.033759595D+03-1.520491112D+00 1.555125152D-02-1.683415215D-05
 8.383557810D-09-1.550875391D-12                1.912920413D+04 3.959395473D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10005.120
-2.133148437D+05-2.953079008D+02 6.876607360D+00-2.102579132D-03 8.596299380D-07
-1.447692760D-10 8.401042790D-15                2.452326136D+04-8.549783749D+00
GeO               Gurvich,1991 pt1 p315 pt2 p274.
 2 tpis91 GE  1.00O   1.00    0.00    0.00    0.00 0   88.6394000      -37694.307
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8782.106
-6.781225630D+03 2.791946972D+02 6.198952860D-01 1.111378013D-02-1.501027092D-05
 1.006783003D-08-2.687101932D-12               -6.711847430D+03 2.156441027D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8782.106
-1.044508485D+06 2.734866048D+03 1.298071298D+00 1.832638634D-03-5.060986350D-07
 6.374958020D-11-2.172371872D-15                -2.362104658D+04 2.350906051D+01
GeO2              Gurvich,1991 pt1 p323 pt2 p278.
 2 tpis91 GE  1.00O   2.00    0.00    0.00    0.00 0  104.6388000    -106171.998
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11258.002
-3.824173830D+03 1.563451633D+02 1.694198285D+00 1.756205059D-02-2.418270032D-05
 1.632388154D-08-4.368957860D-12                -1.477534880D+04 1.556926515D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11258.002
-1.727347526D+05-2.961154443D+02 7.720726250D+00-8.824933390D-05 1.949874702D-08
-2.235834829D-12 1.036128507D-16                -1.387983288D+04-1.669845695D+01
GeS               Gurvich,1991 pt1 p344 pt2 p297.
 2 tpis91 GE  1.00S   1.00    0.00    0.00    0.00 0  104.7050000       92525.110
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9141.110
 3.661018430D+04-5.659653500D+02 6.152936410D+00-2.746908039D-03 2.733435196D-06
-1.460209187D-09 3.278709470D-13                1.274175754D+04-7.705659460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9141.110
-2.351367441D+06 7.211581860D+03-4.362526310D+00 5.451737750D-03-1.721002774D-06
 2.632908084D-10-1.394374040D-14                -3.583317250D+04 6.505566891D+01
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Appendix D (*continued*)

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GeS2              Gurvich,1991 pt1 p347 pt2 p299.
 2 tpis91 GE  1.00S   2.00    0.00    0.00    0.00 0  136.7700000     118817.831
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13067.831
 5.543683600D+04-1.024826697D+03 1.057594552D+01-5.287883910D-03 5.295803080D-06
-2.872529530D-09 6.519027550D-13                 1.735579668D+04-2.991719536D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13067.831
-8.970980360D+04-3.364377000D+01 7.525433720D+00-1.026368137D-05 2.282230718D-09
-2.628748770D-13 1.222218614D-17                 1.195232103D+04-1.135170616D+01
Ge2               Gurvich,1991 pt1 p313 pt2 p273.
 2 tpis91 GE  2.00    0.00    0.00    0.00    0.00 0  145.2800000     471498.929
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10696.129
 2.161978929D+05-3.079621733D+03 1.888047728D+01-2.604825861D-02 2.279151350D-05
-9.028351270D-09 1.146806387D-12                 7.032402550D+04-7.901095968D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10696.129
 1.969461258D+06-5.248687100D+03 1.058277303D+01-3.336551510D-03 1.052745838D-06
-1.484534793D-10 7.475431760D-15                 8.925665990D+04-3.750233948D+01
H                 D0(H2):Herzberg,1970. Moore,1972. Gordon,1999.
 3 g 6/97 H   1.00    0.00    0.00    0.00    0.00 0    1.0079400     217998.828
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.547370801D+04-4.466828530D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 6.078774250D+01-1.819354417D-01 2.500211817D+00-1.226512864D-07 3.732876330D-11
-5.687744560D-15 3.410210197D-19                 2.547486398D+04-4.481917770D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.173757694D+08-1.312035403D+05 3.399174200D+01-3.813999680D-03 2.432854837D-07
-7.694275540D-12 9.644105630D-17                 1.067638086D+06-2.742301051D+02
H+                IP(H): Moore,1972. Gordon,1999.
 3 g10/00 H   1.00E  -1.00    0.00    0.00    0.00 0    1.0073914    1536245.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.840214877D+05-1.140646644D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.840214877D+05-1.140646644D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.840214877D+05-1.140646644D+00
H-                Hotop,1985. Gordon,1999.
 3 g 9/96 H   1.00E   1.00    0.00    0.00    0.00 0    1.0084886     139031.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.597615494D+04-1.139013868D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.597615494D+04-1.139013868D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.597615494D+04-1.139013868D+00
HALO              Gurvich,1996a pt1 p147 pt2 p111.
 2 tpis96 AL  1.00O   1.00H   1.00    0.00    0.00 0   43.9888780       1821.114
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9935.217
 2.668671568D+04-4.663214590D+02 5.383800210D+00 2.902425002D-03-2.243677610D-07
-1.516294323D-09 6.951737660D-13                 1.235914473D+03-6.508837520D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9935.217
 7.847467050D+04-1.515628850D+03 8.572776230D+00-4.142611440D-04 8.935081700D-08
-1.007036446D-11 4.608017250D-16                 6.663241890D+03-2.672948642D+01
HALO2             Gurvich,1996a pt1 p148 pt2 p112.
 2 tpis96 H   1.00AL  1.00O   2.00    0.00    0.00 0   59.9882780    -355473.551
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11980.604
 3.544598910D+03 1.159819104D+02 8.637970690D-01 2.460875785D-02-3.423160120D-05
 2.373182987D-08-6.467608830D-12                -4.449506140D+04 2.012317065D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11980.604
 6.985705440D+05-2.864935042D+03 1.086721494D+01-5.368312700D-05-2.836877559D-08
 6.291641190D-12-3.889033110D-16                -2.764392495D+04-3.775886340D+01
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HBO               Boron oxide-hydride Gurvich,1996  pt1 p39,pt2 p23.
 2 tpis96 H   1.00B   1.00O   1.00    0.00    0.00 0   27.8183400    -210621.205
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9166.898
 6.360975030D+04-8.001557590D+02 6.218816130D+00-7.801679980D-04 3.141286759D-06
-2.031853478D-09 3.738552890D-13                -2.240282910D+04-1.326952393D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9166.898
 8.861860230D+05-3.913068050D+03 9.888644800D+00-8.222269140D-04 1.621530554D-07
-1.703550237D-11 7.372740020D-16                -3.161852029D+03-4.036812720D+01
HBO+              Chase,1998 p223 12/75.
 3 g 1/01 H   1.00B   1.00O   1.00E  -1.00    0.00 0   27.8177914    1175219.729
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9094.629
 6.524471470D+04-7.047337360D+02 5.294271870D+00 1.308494598D-03 2.088343622D-06
-2.564100339D-09 8.198981250D-13                 1.439293436D+05-6.816749230D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9094.629
 1.836083606D+04-1.212975446D+03 6.822901960D+00 9.142272500D-04-2.665355457D-07
 3.297049810D-11-1.530684082D-15                 1.463617504D+05-1.699646159D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9094.629
-2.428406068D+07 1.188114816D+04 5.641928570D+00 1.354130653D-04-2.943428505D-09
-3.120357467D-14 1.432576207D-18                 3.883449210D+04-3.069802126D+00
HBO2              Gurvich,1996a pt1 p42 pt2 p26.
 2 tpis96 H   1.00B   1.00O   2.00    0.00    0.00 0   43.8177400    -560210.053
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10918.102
 6.225087470D+03 7.566153690D+01 1.253406833D+00 1.748006535D-02-1.982688351D-05
 1.229656460D-08-3.153609847D-12                -6.878588780D+04 1.767793507D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10918.102
 1.049369185D+06-4.479145480D+03 1.197755861D+01-4.735743400D-04 6.080207140D-08
-3.641565440D-12 6.155973170D-17                -4.221149470D+04-4.911366820D+01
HBS               Chase,1998 p227 12/75. Jacox,1994.
 2 g 2/01 H   1.00B   1.00S   1.00    0.00    0.00 0   43.8839400     50208.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9286.259
 5.649966210D+04-5.466409950D+02 3.636458390D+00 9.963657670D-03-1.395090386D-05
 1.032834167D-08-3.047186722D-12                 7.919860530D+03 1.182455314D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9286.259
-2.021836183D+05-5.052026620D+02 6.415218280D+00 1.049432932D-03-3.683146690D-07
 5.342968310D-11-2.154140451D-15                 6.485475620D+03-1.331379864D+01
HBS+              Chase,1998 p228 12/75. Jacox,1998 p141.
 3 g 1/01 H   1.00B   1.00S   1.00E  -1.00    0.00 0   43.8833914    1129458.967
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10135.990
 1.489509163D+05-1.847661736D+03 1.147458020D+01-9.476828370D-03 1.110746739D-05
-6.175558610D-09 1.336853512D-12                 1.437822395D+05-4.113512498D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10135.990
 6.610658360D+05-2.791498527D+03 9.131267640D+00-5.063795290D-04 7.751213140D-08
-4.191132930D-12 2.687149095D-17                 1.510734114D+05-3.081426166D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10135.990
-9.547637920D+06 7.401763110D+03 4.866419360D+00 4.143886550D-04-2.488064459D-08
 6.972990680D-13-7.714953540D-18                 7.555300990D+04 3.822638009D+00
HBr               Gurvich,1989 pt1 p205 pt2 p106.
 2 tpis89 H   1.00BR  1.00    0.00    0.00    0.00 0   80.9119400    -36290.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8648.104
 2.527222498D+04-4.065110270D+02 6.043116610D+00-7.717882870D-03 1.149123213D-05
-7.293633280D-09 1.747406491D-12                -3.510414550D+03-9.903186290D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8648.104
 1.170033949D+06-3.786521010D+03 7.503148050D+00-1.284963943D-03 3.206257190D-07
-3.444925160D-11 1.126758417D-15                 1.856413349D+04-2.562712911D+01
HCN               Hf: East,1993. Gurvich,1991 pt1 p226.
 2 g 6/01 H   1.00C   1.00N   1.00    0.00    0.00 0   27.0253400    133082.460
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9235.463
 9.098286930D+04-1.238657512D+03 8.721307870D+00-6.528242940D-03 8.872700830D-06
-4.808886670D-09 9.317898500D-13                 2.098915450D+04-2.746678076D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9235.463
 1.236889278D+06-4.446732410D+03 9.738874850D+00-5.855182640D-04 1.072791440D-07
-1.013313244D-11 3.348247980D-16                 4.221513770D+04-4.005774072D+01
HCO               Hf:Terentis,1996. Jacox,1998 p146.
 2 g 1/01 H   1.00C   1.00O   1.00    0.00    0.00 0   29.0180400     42397.850
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9989.450
-1.189851887D+04 2.151536111D+02 2.730224028D+00 1.806516108D-03 4.984300570D-06
-5.814567920D-09 1.869689894D-12                 2.905755640D+03 1.136772540D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9989.450
 6.949606120D+05-3.656223380D+03 9.604731170D+00-1.117129278D-03 2.875328019D-07
-3.626247740D-11 1.808329595D-15                 2.543704440D+04-3.582473720D+01
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Appendix D (*continued*)

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HCO+                Formyl ion. Hf:Chase,1998 p603 12/70. Jacox,1998 p145.
 3 g 1/01 H   1.00C   1.00O   1.00E  -1.00     0.00 0    29.0174914      833034.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9045.992
 1.573442506D+05-1.867692159D+03 1.099235423D+01-1.211637888D-02 1.659091514D-05
-1.016592642D-08 2.391234771D-12                 1.084930280D+05-4.078261620D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9045.992
 1.219060653D+06-4.714294890D+03 1.021192493D+01-8.854517070D-04 1.667408026D-07
-1.683285548D-11 7.040051780D-16                 1.277989027D+05-4.351158460D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9045.992
-4.593151930D+05-1.132568857D+03 7.739065200D+00-2.648464060D-05 1.613280824D-09
-5.113217500D-14 6.588027500D-19                 1.032813937D+05-2.458716820D+01
HCCN                Gurvich,1989 pt1 p228 pt2 p216.
 2 tpis89 H   1.00C   2.00N   1.00     0.00     0.00 0    39.0360400      610430.628
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11865.731
 2.994114377D+03-4.404660680D+02 6.940036410D+00 3.846304960D-03-1.264728529D-06
-3.639235130D-10 2.748929104D-13                 7.370878640D+04-1.315302591D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11865.731
 9.395620310D+05-4.091067750D+03 1.272233302D+01-6.874405310D-04 1.231169968D-07
-1.186956238D-11 4.760610350D-16                 9.585164820D+04-5.248695794D+01
HCCO                Ketenyl rad. Osborn,1997. Szalay,1996. Jacox,1998 p156.
 2 g 6/01 H   1.00C   2.00O   1.00     0.00     0.00 0    41.0287400      176568.100
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11664.994
 6.959612700D+04-1.164594402D+03 9.456616260D+00-2.331240632D-03 5.161873600D-06
-3.526169970D-09 8.599143230D-13                 2.535003992D+04-2.726355351D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11664.994
 1.093922002D+06-4.498228210D+03 1.246446433D+01-6.343317400D-04 1.108549019D-07
-1.125488678D-11 5.689151940D-16                 4.652280300D+04-5.099070430D+01
HCL                 Gurvich,1989 pt1 p186 pt2 p93.
 2 tpis89 H   1.00CL  1.00     0.00     0.00     0.00 0    36.4609400      -92310.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8640.104
 2.062588287D+04-3.093368855D+02 5.275418850D+00-4.828874220D-03 6.195794600D-06
-3.040023782D-09 4.916790030D-13                -1.067782299D+04-7.309305408D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8640.104
 9.157749510D+05-2.770550211D+03 5.973539790D+00-3.629810060D-04 4.735529190D-08
 2.810262054D-12-6.656104220D-16                 5.674958050D+03-1.642825822D+01
HD                  Gurvich,1989 pt1 p144 pt2 p53.
 3 tpis89 H   1.00D   1.00     0.00     0.00     0.00 0     3.0220420        323.302
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8509.102
 2.519120338D+04-2.761004999D+02 4.644441290D+00-2.082376844D-03 1.418070803D-06
 2.839893835D-10-3.202331030D-13                 3.913616430D+02-9.395396120D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8509.102
 8.455830000D+05-1.956578537D+03 4.404373870D+00 5.751681090D-04-2.131983152D-07
 4.036126680D-11-2.727170705D-15                 1.227254163D+04-1.084742878D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8509.102
 4.829960940D+08-3.077144916D+05 7.864816510D+01-8.332990910D-03 4.732254110D-07
-1.372721571D-11 1.614120677D-16                 2.431070386D+06-6.569437060D+02
HD+                 Chase,1998 p1034.
 3 j 9/77 H   1.00D   1.00E  -1.00     0.00     0.00 0     3.0214934    1496792.618
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8614.000
-8.070073050D+04 8.796432580D+02 5.968932160D-02 5.418181010D-03-2.021515155D-06
-4.945261650D-10 4.092935650D-13                 1.744992497D+05 1.934281193D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8614.000
 1.340083030D+06-5.730069570D+03 1.213836576D+01-5.243338120D-03 1.976302344D-06
-3.306573530D-10 1.937902763D-14                 2.135348051D+05-6.128758390D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8614.000
 6.116880040D+06-1.884939608D+04 1.741572175D+01-2.495631471D-03 1.746560021D-07
-5.815870420D-12 7.638706130D-17                 3.018292196D+05-1.105093671D+02
HDO                 Gurvich,1989 pt1 p145 pt2 p55.
 2 g 5/99 H   1.00D   1.00O   1.00     0.00     0.00 0    19.0214420     -245280.477
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9925.723
-2.737795356D+04 4.310503900D+02 1.558479899D+00 5.764969150D-03-4.855129360D-06
 3.382990170D-09-1.040863879D-12                -3.273226450D+04 1.487751891D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9925.723
 1.711376798D+06-5.322872300D+03 9.124351520D+00-3.400664150D-04 4.152343520D-08
-4.780768570D-14-1.468035170D-16                 3.245224680D+03-3.774600680D+01
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HDO2              Gurvich,1989 pt1 p146 pt2 p56.
 2 g 5/99 H   1.00D   1.00O   2.00     0.00     0.00 0   35.0208420     -140241.635
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11334.965
-3.216476650D+04 7.492334460D+02-1.957676212D+00 2.412802791D-02-2.915946684D-05
 1.930016324D-08-5.226986310D-12                 -2.151059175D+04 3.672406740D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11334.965
 1.313180619D+06-5.175637120D+03 1.216490975D+01-6.136699480D-04 1.227560176D-07
-1.079624939D-11 3.874013720D-16                  1.303209670D+04-5.085276870D+01
HF                Gurvich,1989 pt1 p162 pt2 p77.
 3 tpis89 H   1.00F   1.00     0.00     0.00     0.00 0   20.0063432     -273300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8599.103
-3.192098970D+03 5.986807720D+01 3.055113902D+00 1.684673783D-03-3.287394830D-06
 3.095923617D-09-9.764691610D-13                 -3.418443160D+04 3.294904120D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8599.103
 7.257089040D+05-1.484797741D+03 3.855527470D+00 7.138989850D-04-2.106757333D-07
 3.050092453D-11-1.639495583D-15                 -2.355456660D+04-3.203856830D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8599.103
 1.764588423D+08-8.789998060D+04 1.886524859D+01-6.850866180D-04-1.403468022D-08
 1.503711045D-12-2.717518148D-17                  6.853573220D+05-1.393231574D+02
HI                Chase,1998 p1265.
 2 j 9/61 H   1.00I   1.00     0.00     0.00     0.00 0  127.9124100      26359.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8656.500
 1.872881730D+04-3.431788840D+02 5.956712430D+00-8.543439600D-03 1.454780274D-05
-1.049104164D-08 2.839734003D-12                  3.682950720D+03-8.149756090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8656.500
 4.724921450D+05-1.923465741D+03 5.758048970D+00-4.066266380D-04 9.474332050D-08
-1.033534431D-11 4.611614790D-16                  1.394857037D+04-1.182487652D+01
HNC               Hf:Gurvich,1991 pt1 p227. Jacox,1998 p145.
 2 g 6/01 H   1.00N   1.00C   1.00     0.00     0.00 0   27.0253400     194378.121
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10000.724
 4.870620640D+04-9.891456250D+02 9.722153890D+00-1.113593916D-02 1.668862707D-05
-1.113940941D-08 2.893600868D-12                  2.664679758D+04-3.104826344D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10000.724
 1.198791660D+06-3.918941860D+03 9.118020090D+00-3.417761100D-04 3.314809680D-08
-5.701574740D-13-7.789455390D-17                  4.658810300D+04-3.468575882D+01
HNCO              Hf:East,1993. Jacox,1998 p236.
 2 g 7/00 H   1.00N   1.00C   1.00O    1.00     0.00 0   43.0247400     -118056.529
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10966.126
 7.542460080D+04-9.550937770D+02 6.725705870D+00 4.705687500D-03-4.959475510D-06
 3.694255120D-09-1.164859121D-12                 -1.068149742D+04-1.365584762D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10966.126
 1.253216926D+06-5.021091540D+03 1.247789314D+01-6.891655250D-04 1.097738448D-07
-9.306403800D-12 3.242606950D-16                  1.453155559D+04-5.306419819D+01
HNO               Gurvich,1989 pt1 p362 pt2 p227. Jacox,1998 p151.
 2 g10/01 H   1.00N   1.00O   1.00     0.00     0.00 0   31.0140400     102032.725
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9941.880
-6.854764860D+04 9.551627200D+02-6.000720210D-01 7.995176750D-03-6.547079160D-07
-3.670513400D-09 1.783392519D-12                  6.435351260D+03 3.048166179D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9941.880
-5.795614980D+06 1.945457427D+04-2.152568374D+01 1.797428992D-02-4.976040670D-06
 6.397924170D-10-3.142619368D-14                 -1.104192372D+05 1.818650338D+02
HNO2              Cis-trans. Gurvich,1989 pt1 p363 pt2 p228.
 2 tpis89 H   1.00N   1.00O   2.00     0.00     0.00 0   47.0134400      -78451.922
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11597.285
 8.591985060D+03 1.203644046D+02 9.412979120D-01 1.942891839D-02-2.253174194D-05
 1.384587594D-08-3.473550460D-12                 -1.106337202D+04 2.073967331D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11597.285
 8.787904130D+05-3.990455030D+03 1.187349269D+01-4.881900610D-04 7.133636790D-08
-5.376303340D-12 1.581778986D-16                  1.246343241D+04-4.608874688D+01
HNO3              Gurvich,1989 pt1 p367 pt2 p231.
 2 g 5/99 H   1.00N   1.00O   3.00     0.00     0.00 0   63.0128400     -133912.869
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11876.390
 9.202869010D+03 1.093774496D+02-4.521042450D-01 2.984914503D-02-3.190635500D-05
 1.720931528D-08-3.782649830D-12                 -1.764048507D+04 2.746644879D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11876.390
-9.497809640D+04-2.733024468D+03 1.449426995D+01-7.821868050D-04 1.702693665D-07
-1.930543961D-11 8.870455120D-16                 -4.882517780D+03-5.928392985D+01
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Appendix D (*continued*)

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HOCL              Hf:Gurvich,1989 pt1 p187. Jacox,1998 p155.
 2 g 1/01 H   1.00O   1.00CL  1.00     0.00     0.00 0    52.4603400      -75740.032
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10224.626
-9.739307430D+03 3.547569520D+02 1.539514254D-01 1.617051795D-02-2.179693631D-05
 1.509103049D-08-4.125383510D-12                 -1.176323791D+04 2.473257759D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10224.626
 8.530457810D+05-2.847760552D+03 7.948329040D+00-1.048782013D-04-1.482405043D-08
 4.591678270D-12-3.060073987D-16                  7.250964950D+03-2.249831690D+01
HOF               Gurvich,1989 pt1 p171 pt2 p79.
 2 tpis89 H   1.00O   1.00F   1.00     0.00     0.00 0    36.0057432      -96898.221
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10088.435
-3.696888300D+04 7.809006660D+02-2.077685317D+00 2.038690173D-02-2.586919999D-05
 1.713797538D-08-4.551281870D-12                 -1.631720064D+04 3.645052500D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10088.435
 8.812018230D+05-3.120013169D+03 8.223710070D+00-2.298036315D-04 1.459115709D-08
 1.095883303D-12-1.404445608D-16                  6.300546710D+03-2.590150427D+01
HO2               Hf:Hills,1984 & NASA data. Jacox,1998 p153.
 2 g 5/99 H   1.00O   2.00     0.00     0.00     0.00 0    33.0067400      12020.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10002.162
-7.598882540D+04 1.329383918D+03-4.677388240D+00 2.508308202D-02-3.006551588D-05
 1.895600056D-08-4.828567390D-12                 -5.873350960D+03 5.193602140D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10002.162
-1.810669724D+06 4.963192030D+03-1.039498992D+00 4.560148530D-03-1.061859447D-06
 1.144567878D-10-4.763064160D-15                 -3.200817190D+04 4.066850920D+01
HO2-              B3LYP.  EA: Oakes, 1985.
 2 g 5/02 H   1.00O   2.00E   1.00     0.00     0.00 0    33.0072886      -97923.080
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10245.320
 1.103839835D+05-1.047963653D+03 6.360013990D+00 2.942520461D-03-6.284141340D-06
 5.438254240D-09-1.647305820D-12 0.000000000D+00-7.417741590D+03-1.251878002D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10245.320
 7.933306000D+05-2.503312417D+03 7.548962330D+00 8.308390150D-05-5.969730910D-08
 9.955377000D-12-5.606477280D-16 0.000000000D+00 2.512079084D+03-2.070065846D+01
HPO               Hf:Gurvich,1989 pt1 p424. Jacox,1994 p46.
 2 tpis89 H   1.00P   1.00O   1.00     0.00     0.00 0    47.9811010      -56868.759
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10065.343
-3.816314120D+04 7.927641870D+02-1.889940652D+00 1.800907425D-02-1.857631793D-05
 1.018768867D-08-2.355583619D-12                 -1.157641240D+04 3.692925910D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10065.343
 3.842459450D+05-2.434951707D+03 8.582173920D+00-4.058448570D-04-1.669488740D-08
 2.253640566D-11-1.943063011D-15                  5.761632120D+03-2.649097544D+01
HSO3F             Chase,1998 p1057.
 2 j 6/72 H   1.00S   1.00O   3.00F   1.00     0.00 0   100.0695432     -753120.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15014.174
 6.896242130D+03-9.305810750D+01 1.570331788D+00 3.780820750D-02-4.872720780D-05
 3.160796011D-08-8.189782930D-12                 -9.180240820D+04 1.716315977D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15014.174
 5.544047080D+05-3.974424320D+03 1.778869264D+01-4.409322030D-04 5.944411390D-08
-3.927015810D-12 8.891284000D-17                 -7.153438270D+04-7.613127849D+01
H2                Ref-Elm. Gurvich,1978 pt1 p103 pt2 p31.
 3 tpis78 H   2.00     0.00     0.00     0.00     0.00 0     2.0158800          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8468.102
 4.078323210D+04-8.009186040D+02 8.214702010D+00-1.269714457D-02 1.753605076D-05
-1.202860270D-08 3.368093490D-12                  2.682484665D+03-3.043788844D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8468.102
 5.608128010D+05-8.371504740D+02 2.975364532D+00 1.252249124D-03-3.740716190D-07
 5.936625200D-11-3.606994100D-15                  5.339824410D+03-2.202774769D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8468.102
 4.966884120D+08-3.147547149D+05 7.984121880D+01-8.414789210D-03 4.753248350D-07
-1.371873492D-11 1.605461756D-16                  2.488433516D+06-6.695728110D+02
H2+               Gurvich,1978 pt1 p107 pt2 p33.
 3 tpis78 H   2.00E  -1.00     0.00     0.00     0.00 0     2.0153314    1494672.430
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8583.103
-3.120886060D+04 2.304622909D+02 3.335564420D+00-2.419056763D-03 7.006022340D-06
-5.610010660D-09 1.564169746D-12                  1.774104638D+05-8.278523760D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8583.103
 1.672225964D+06-6.595184990D+03 1.279321925D+01-5.509345260D-03 2.030669412D-06
-3.351027480D-10 1.946089104D-14                  2.189999548D+05-6.792710780D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8583.103
-1.822070983D+08 1.018196269D+05-1.245831898D+01 1.076647496D-03-3.932290360D-08
 6.285405030D-13-2.094721880D-18                 -6.513101500D+05 1.471415370D+02
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H2-                Chase,1998 p1312.
 2 j 9/77 H   2.00E   1.00     0.00     0.00     0.00 0     2.0164286      235168.362
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8620.592
-9.753565670D+04 1.221166236D+03-2.264588838D+00 1.237202227D-02-1.127100020D-05
 5.367239950D-09-1.049420160D-12                  2.121399948D+04 3.050556136D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8620.592
 9.599275620D+04-9.144682880D+02 5.149418810D+00-1.016559478D-04 5.446919560D-08
-6.155174450D-12 2.822451181D-16                  3.234105180D+04-1.440780980D+01
HBOH               Gurvich,1996a pt1 p44 pt2 p27.
 2 g 9/98 H   2.00B   1.00O    1.00     0.00     0.00 0    28.8262800      -48724.364
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10940.536
-6.159644190D+04 1.223483035D+03-5.460370510D+00 3.555388680D-02-4.675020140D-05
 3.236008850D-08-8.986053320D-12                 -1.263659051D+04 5.422352290D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10940.536
 1.534611049D+06-5.753666430D+03 1.270893665D+01-7.059628250D-04 1.027679375D-07
-7.670926740D-12 2.211854768D-16                  2.779370419D+04-5.608860080D+01
HCHO,formaldehy    Hf:TRC(6/78) w-5300. Gurvich,1991 pt1 p62 pt2 p47.
 2 g 5/01 H   2.00C   1.00O    1.00     0.00     0.00 0    30.0259800     -108580.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10019.717
-1.173916343D+05 1.873628846D+03-6.890288570D+00 2.641561665D-02-2.186389299D-05
 1.005693006D-08-2.023476949D-12                 -2.307351768D+04 6.420420550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10019.717
 1.700825405D+06-7.620853840D+03 1.472447547D+01-1.649111754D-03 3.292144720D-07
-3.495049770D-11 1.526135000D-15                  3.146812947D+04-7.386478500D+01
HCOOH              Formic acid. Chao,1978.
 2 g 6/01 H   2.00C   1.00O    2.00     0.00     0.00 0    46.0253800     -378570.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10927.649
-2.906279097D+04 7.658378880D+02-3.328414130D+00 2.817542991D-02-2.370050804D-05
 1.166063663D-08-2.791373170D-12                 -5.006443470D+04 4.387094230D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10927.649
 4.872336450D+05-7.632238080D+03 2.132788153D+01-4.402546540D-03 1.102001695D-06
-1.364343517D-10 6.648429750D-15                 -5.781431910D+03-1.111790688D+02
H2F2               Gurvich,1989  v1 pt1 p164 pt2 p308.
 2 tpis89 H   2.00F   2.00     0.00     0.00     0.00 0    40.0126864     -569923.778
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13869.430
 5.259214710D+04-9.913544890D+02 1.043577115D+01-2.407796033D-03-6.376956160D-07
 2.735784900D-09-1.104348590D-12                 -6.572460830D+04-3.038432132D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13869.430
 1.464995601D+06-3.335074920D+03 9.187487040D+00 1.051127249D-03-3.278605570D-07
 4.456046230D-11-2.281370136D-15                 -4.825442090D+04-2.639128168D+01
H2O                Hf:Cox,1989. Woolley,1987. TRC(10/88) tuv25.
 2 g 8/89 H   2.00O   1.00     0.00     0.00     0.00 0    18.0152800     -241826.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9904.092
-3.947960830D+04 5.755731020D+02 9.317826530D-01 7.222712860D-03-7.342557370D-06
 4.955043490D-09-1.336933246D-12                 -3.303974310D+04 1.724205775D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9904.092
 1.034972096D+06-2.412698562D+03 4.646110780D+00 2.291998307D-03-6.836830480D-07
 9.426468930D-11-4.822380530D-15                 -1.384286509D+04-7.978148510D+00
H2O+               Gurvich,1989 pt1 p125 pt2 p38.
 3 tpis89 H   2.00O   1.00E   -1.00     0.00     0.00 0    18.0147314      981601.766
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9934.466
-1.753892720D+03 2.249850054D+02 1.989400675D+00 6.117895160D-03-7.095436640D-06
 5.547659470D-09-1.704344789D-12                  1.159585952D+05 1.135409642D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9934.466
 6.228714260D+05-2.864257487D+03 7.717565560D+00-9.027801670D-04 6.177436860D-07
-1.201457479D-10 7.407709940D-15                  1.342086651D+05-2.636617920D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9934.466
-2.040922112D+07-1.072691716D+03 1.131977392D+01-7.364445000D-04 5.416450200D-08
-1.900872342D-12 2.604761558D-17                  1.042565942D+05-5.467272320D+01
H2O2               Hf:Gurvich,1989 pt1 p127. Gurvich,1978 pt1 p121.
 2 g 6/99 H   2.00O   2.00     0.00     0.00     0.00 0    34.0146800     -135880.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11158.835
-9.279533580D+04 1.564748385D+03-5.976460140D+00 3.270744520D-02-3.932193260D-05
 2.509255235D-08-6.465045290D-12                 -2.494004728D+04 5.877174180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11158.835
 1.489428027D+06-5.170821780D+03 1.128204970D+01-8.042397790D-05-1.818383769D-08
 6.947265590D-12-4.827831900D-16                  1.418251038D+04-4.650855660D+01
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Appendix D (*continued*)

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H2S               Gurvich,1989 pt1 p298 pt2 p181.
 2 g 4/01 H   2.00S   1.00    0.00    0.00    0.00 0   34.0808800     -20600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9958.421
 9.543808810D+03-6.875175080D+01 4.054921960D+00-3.014557336D-04 3.768497750D-06
-2.239358925D-09 3.086859108D-13               -3.278457280D+03 1.415194691D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9958.421
 1.430040220D+06-5.284028650D+03 1.016182124D+01-9.703849960D-04 2.154003405D-07
-2.169695700D-11 9.318163070D-16                2.908696214D+04-4.349160391D+01
H2SO4             Gurvich,1989 pt1 p300 pt2 p182.
 2 tpis89 H   2.00S   1.00O   4.00    0.00    0.00 0   98.0784800     -732731.721
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16508.589
-4.129150050D+04 6.681589890D+02-2.632753507D+00 5.415382480D-02-7.067502230D-05
 4.684611420D-08-1.236791238D-11               -9.315660120D+04 3.961096201D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16508.589
 1.437877914D+06-6.614902530D+03 2.157662058D+01-4.806255970D-04 3.010775121D-08
 2.334842469D-12-2.946330375D-16               -5.259092950D+04-1.023603724D+02
H2BOH             Gurvich,1996a pt1 p46 pt2 p29.
 2 tpis96 H   3.00B   1.00O   1.00    0.00    0.00 0   29.8342200     -289633.898
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10622.306
-8.686766780D+04 1.820335089D+03-1.032373881D+01 4.922801060D-02-5.978619910D-05
 3.946062730D-08-1.068442257D-11               -4.415238150D+04 7.986177290D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10622.306
 2.294795193D+06-9.382923560D+03 1.798228329D+01-1.506116214D-03 2.635641095D-07
-2.483163637D-11 9.736759120D-16                2.039738953D+04-9.448201210D+01
HB(OH)2           Gurvich,1996a pt1 p47 pt2 p30.
 2 tpis96 H   3.00B   1.00O   2.00    0.00    0.00 0   45.8336200     -644438.724
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12157.532
-2.067044022D+04 9.534459160D+02-8.088956520D+00 5.972425290D-02-8.071336320D-05
 5.612118350D-08-1.553607566D-11               -8.264270810D+04 6.539571640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12157.532
 2.122674609D+06-8.615948940D+03 1.966179520D+01-8.148411500D-04 8.955082040D-08
-3.344830510D-12-6.919578140D-17               -2.788790377D+04-9.983559610D+01
H3BO3             Gurvich,1996a pt1 p50 pt2 p32.
 2 tpis96 H   3.00B   1.00O   3.00    0.00    0.00 0   61.8330200    -1004360.442
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13559.958
 2.568901843D+04 1.138029495D+02-4.045096580D+00 5.924521680D-02-8.148028410D-05
 5.658593290D-08-1.549277050D-11               -1.221702050D+05 4.132220140D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13559.958
 2.297369132D+06-8.933571790D+03 2.193496552D+01-3.094783490D-04-5.064052990D-08
 1.482296684D-11-9.764420900D-16               -6.970298470D+04-1.122292829D+02
H3B3O3            Gurvich,1996a pt1 p53 pt2 p34.
 2 tpis96 H   3.00B   3.00O   3.00    0.00    0.00 0   83.4550200    -1203760.987
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15603.321
-1.985284188D+05 4.104132090D+03-2.827215617D+01 1.269639253D-01-1.558505781D-04
 9.966304070D-08-2.603677650D-11               -1.648494375D+05 1.763917407D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15603.321
 1.286220713D+06-1.093258784D+04 3.213518670D+01-2.595402269D-03 5.353766470D-07
-5.833567380D-11 2.600757913D-15               -8.752856890D+04-1.770847815D+02
H3B3O6            Gurvich,1996a pt1 p55 pt2 p35.
 2 tpis96 H   3.00B   3.00O   6.00    0.00    0.00 0  131.4532200    -2263687.611
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23696.853
-2.067031503D+04 7.083391540D+02-7.123820950D+00 1.025049979D-01-1.295004602D-04
 8.322737590D-08-2.145746724D-11               -2.778049216D+05 6.063597630D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23696.853
 1.952433352D+06-1.154932896D+04 3.892676110D+01-1.113852280D-03 1.280317726D-07
-5.728464820D-12-2.214529572D-17               -2.120927136D+05-2.075566801D+02
H3F3              Gurvich,1989 pt1 p166 pt2 p309.
 2 tpis89 H   3.00F   3.00    0.00    0.00    0.00 0   60.0190296     -883676.790
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15263.022
 9.888562650D+04-1.380212880D+03 8.980458470D+00 1.871609057D-02-3.127862508D-05
 2.589436165D-08-8.040372270D-12               -1.013661491D+05-2.585302557D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15263.022
 2.515790373D+06-8.789423320D+03 2.023933445D+01-1.131704646D-03 1.692779921D-07
-1.308662105D-11 3.978322000D-16               -5.471713650D+04-9.907787640D+01
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H3O+                Gurvich,1989 pt1 p130 pt2 p41.
 3 tpis89 H   3.00O   1.00E  -1.00    0.00    0.00 0   19.0226714     598000.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10046.427
-6.447640150D+04 1.181817922D+03-3.801893060D+00 2.220628313D-02-2.445343237D-05
 1.573297747D-08-4.158836410D-12                 6.530613320D+04 4.282723130D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10046.427
 2.955126200D+06-9.185669410D+03 1.341398696D+01-5.590339210D-04 1.138387119D-08
 7.259927210D-12-6.133734360D-16                 1.290534257D+05-7.021828180D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10046.427
-1.591228592D+07 4.898727210D+03 8.881336820D+00 1.299244015D-04-8.169245590D-09
 2.649115685D-13-3.472865280D-18                 2.090178405D+04-3.217683350D+01
(HCOOH)2            Formic acid dimer. Chao,1978.
 2 g 6/01 H   4.00C   2.00O   4.00    0.00    0.00 0   92.0507600    -820942.640
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19631.909
-2.001447991D+05 3.502457370D+03-1.853488051D+01 9.547467130D-02-1.059184484D-04
 6.323086900D-08-1.567561216D-11                -1.172621688D+05 1.319646887D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19631.909
 3.308188420D+06-1.633668256D+04 3.751348820D+01-3.148108995D-03 6.008707760D-07
-6.144462500D-11 2.600562474D-15                -6.265894440D+03-2.107476941D+02
H4F4                Gurvich,1989 pt1 p167 pt2 p310.
 2 tpis89 H   4.00F   4.00    0.00    0.00    0.00 0   80.0253728   -1186932.336
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21654.080
 1.315109024D+05-1.840361560D+03 1.264093152D+01 2.495407360D-02-4.170394610D-05
 3.452523840D-08-1.072034360D-11                -1.364003454D+05-4.122913530D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21654.080
 3.354037990D+06-1.171922040D+04 2.765243565D+01-1.508934621D-03 2.257027572D-07
-1.744867255D-11 5.304351740D-16                -7.420213160D+04-1.388603332D+02
H5F5                Gurvich,1989 pt1 p168 pt2 p311.
 2 tpis89 H   5.00F   5.00    0.00    0.00    0.00 0  100.0317160   -1490187.882
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28045.138
 1.641361897D+05-2.300510396D+03 1.630140545D+01 3.119205422D-02-5.212926350D-05
 4.315611240D-08-1.340031413D-11                -1.714345408D+05-5.682157380D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28045.138
 4.192290730D+06-1.464903043D+04 3.506554920D+01-1.886170471D-03 2.821289954D-07
-2.181090984D-11 6.630474160D-16                -9.368704200D+04-1.788592044D+02
H6F6                Gurvich,1989 pt1 p169 pt2 p312.
 2 tpis89 H   6.00F   6.00    0.00    0.00    0.00 0  120.0380592   -1805545.131
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         34334.493
 1.956886618D+05-2.753909880D+03 1.975625055D+01 3.807717010D-02-6.341218880D-05
 5.219233290D-08-1.612185649D-11                -2.079269410D+05-7.113607980D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         34334.493
 5.024520320D+06-1.742817868D+04 4.214870500D+01-2.084564791D-03 2.930051519D-07
-2.052079159D-11 5.206937300D-16                -1.154497653D+05-2.163947001D+02
H7F7                Gurvich,1989 pt1 p170 pt2 p313.
 2 tpis89 H   7.00F   7.00    0.00    0.00    0.00 0  140.0444024   -2099698.974
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         40827.254
 2.293867477D+05-3.220807860D+03 2.362235212D+01 4.366801880D-02-7.297990340D-05
 6.041786420D-08-1.876025627D-11                -2.418637479D+05-8.838812260D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         40827.254
 5.868789830D+06-2.050863473D+04 4.989176110D+01-2.640634895D-03 3.949796330D-07
-3.053515088D-11 9.282601780D-16                -1.330177809D+05-2.592385142D+02
He                  Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 5/97 HE  1.00    0.00    0.00    0.00    0.00 0    4.0026020          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 9.287239740D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 9.287239740D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 3.396845420D+06-2.194037652D+03 3.080231878D+00-8.068957550D-05 6.252784910D-09
-2.574990067D-13 4.429960218D-18                 1.650518960D+04-4.048814390D+00
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He+                Moore,1971; Moore,1970a. Gordon,1999.
 3 g 3/97 HE  1.00E  -1.00    0.00    0.00    0.00 0    4.0020534    2378521.473
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.853233739D+05 1.621665557D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.853233739D+05 1.621665557D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.853233739D+05 1.621665557D+00
Hg                 Hf:Cox,1989. Moore,1971. Gordon,1999.
 3 g 1/98 HG  1.00    0.00    0.00    0.00    0.00 0  200.5900000      61380.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 6.636900080D+03 6.800201540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 5.146573510D+04-1.681269855D+02 2.718343098D+00-1.445026192D-04 5.158977660D-08
-9.472485010D-12 7.034797406D-16                 7.688684930D+03 5.271236090D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 5.358443930D+08-4.433853810D+05 1.463223992D+02-2.318441669D-02 1.916335174D-06
-7.419662000D-11 1.067224054D-15                 3.391999920D+06-1.201225990D+03
Hg+                Moore,1971. Gordon,1999.
 3 g 7/97 HG  1.00E  -1.00    0.00    0.00    0.00 0  200.5894514    1074643.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21                 1.285037483D+05 7.493344500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.229984728D+04 2.732269908D+01 2.484182160D+00-4.426797610D-06 7.489685860D-09
-2.549887287D-12 2.819873366D-16                 1.283188257D+05 7.625244570D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-5.498617710D+07 3.775543500D+04-7.155545550D+00 1.170310234D-03-7.931471440D-08
 4.029174000D-12-7.741071633D-17                -1.676894201D+05 9.116750020D+01
HgBr2              Hf: Pankratz,1984. Chase,1998 p485 3/62.
 2 g12/00 HG  1.00BR  2.00    0.00    0.00    0.00 0  360.3980000     -91311.616
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15658.384
-1.991826537D+03-1.902186083D+02 8.246401260D+00-1.607089392D-03 1.947654549D-06
-1.242873546D-09 3.241818310D-13                -1.230723096D+04-8.716659300D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15658.384
-2.243649290D+04-3.312652270D+00 7.502765170D+00-1.202360213D-06 2.830526999D-10
-3.407686700D-14 1.640497921D-18                -1.327483366D+04-4.368555600D+00
I                  Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 3/97 I   1.00    0.00    0.00    0.00    0.00 0  126.9044700     106760.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.698199675D+02-2.716437233D+00 2.517385557D+00-5.730692070D-05 1.031716184D-07
-9.670641930D-11 3.706471651D-14                 1.210750090D+04 7.405823130D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-7.785860570D+05 2.303279568D+03 2.886686091D-03 1.180878463D-03-2.264074866D-07
 1.963511339D-11-6.243525941D-16                -2.616792742D+03 2.558922997D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.747630780D+07-8.681111190D+04 3.950617020D+01-6.514063250D-03 5.380695340D-07
-1.969145066D-11 2.643177163D-16                 6.384843030D+05-2.972997119D+02
I+                 Moore,1971. Moore,1970a. Gordon,1999.
 3 g10/97 I   1.00E  -1.00    0.00    0.00    0.00 0  126.9039214    1121351.028
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-8.014969010D+02 8.139052610D+00 2.470174760D+00 4.161393820D-05 7.133397860D-09
-7.105950140D-11 4.873766102D-14                 1.340794213D+05 7.903420090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-7.788385330D+05 2.404962651D+03-1.791751142D-01 1.227311979D-03-1.801494030D-07
 9.923983960D-12-9.775286439D-17                 1.188531631D+05 2.710544347D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-6.314420010D+08 3.971131910D+05-9.860191990D+01 1.358236563D-02-9.920747650D-07
 3.684927700D-11-5.301687095D-16                -3.001474591D+06 8.790468740D+02
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Appendix D (*continued*)

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I-                Hotop,1985. Gordon,1999.
 3 g10/97 I   1.00E   1.00     0.00     0.00     0.00 0  126.9050186     -194595.572
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.414970936D+04 6.113465380D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.414970936D+04 6.113465380D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.414970936D+04 6.113465380D+00
IF5               Gurvich,1989 pt1 p232 pt2 p123.
 2 tpis89 I   1.00F   5.00     0.00     0.00     0.00 0  221.8964860     -841000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20044.142
 2.026184530D+05-3.598183170D+03 2.530349738D+01-1.348602458D-02 1.105687229D-05
-4.707939510D-09 7.864411470D-13                -8.700147250D+04-1.112719941D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20044.142
-3.620506260D+05-1.639236093D+02 1.612272743D+01-4.914431550D-05 1.086015052D-08
-1.244672691D-12 5.763593620D-17                -1.061642293D+05-5.398773360D+01
IF7               Gurvich,1989 pt1 p234 pt2 p124.
 2 tpis89 I   1.00F   7.00     0.00     0.00     0.00 0  259.8932924     -961500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24123.333
 2.999853564D+05-5.501554130D+03 3.627133980D+01-2.095765818D-02 1.761972680D-05
-7.829142330D-09 1.405939372D-12                -9.331307660D+04-1.754216150D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24123.333
-5.614422640D+05-2.646288326D+02 2.219879891D+01-7.984221470D-05 1.768835964D-08
-2.031523755D-12 9.423767390D-17                -1.225245322D+05-8.774010730D+01
I2                Gurvich,1989 pt1 p220 pt2 p117.
 2 tpis89 I   2.00     0.00     0.00     0.00     0.00 0  253.8089400      62420.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10116.122
-5.087968770D+03-1.249585210D+01 4.504219090D+00 1.370962533D-04-1.390523014D-07
 1.174813853D-10-2.337541043D-14                 6.213469810D+03 5.583836940D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10116.122
-5.632594160D+06 1.793961560D+04-1.723055169D+01 1.244214080D-02-3.332768580D-06
 4.125477940D-10-1.960461713D-14                -1.068505292D+05 1.600531883D+02
In                Hf:Gurvich,1996a. Johansson,1966. Moore,1971. Gordon,1999.
 3 g 1/99 IN  1.00     0.00     0.00     0.00     0.00 0  114.8180000     240700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6198.649
 5.149518050D+04-9.177999020D+02 8.938687950D+00-2.224112602D-02 3.823881940D-05
-2.890116948D-08 8.047481221D-12                 3.239031620D+04-2.764567028D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6198.649
-1.683608899D+06 2.210473186D+03 3.472219370D+00-1.082267422D-03 3.479699980D-07
-5.158092410D-11 3.183043089D-15                 1.095965206D+04 2.557189088D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6198.649
-2.289146601D+06 3.908691060D+04-1.789204885D+01 3.655375250D-03-2.576493626D-07
 7.929188320D-12-9.066642170D-17                -2.376257502D+05 1.738048645D+02
In+               IP:Johansson,1966. Moore,1971. Gordon,1999.
 3 g 4/99 IN  1.00E  -1.00     0.00     0.00     0.00 0  114.8174514      6996.425
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 2.150488908D-01-2.523854672D-03 2.500011877D+00-2.869063919D-08 3.753870400D-11
-2.525942419D-14 6.842932660D-18                 9.610930170D+01 5.963254400D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 4.536995140D+04-1.445142103D+02 2.681812441D+00-1.157480060D-04 3.947714810D-08
-6.879243620D-12 4.819204920D-16                 1.004261440D+03 4.683759180D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-6.188028020D+07 1.322640301D+04 7.453303840D+00-1.893250634D-03 2.114636410D-07
-8.432019810D-12 1.185570972D-16                -1.335858982D+05-2.765870435D+01
InBr              Gurvich,1996a pt1 p291 pt2 p233
 2 tpis96 IN  1.00BR  1.00     0.00     0.00     0.00 0  194.7220000      -54115.879
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10084.121
-2.540851435D+03-5.294704710D+01 4.717438090D+00-4.344669490D-04 6.513513640D-07
-4.403995150D-10 1.234046209D-13                -7.607594280D+03 4.258881000D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10084.121
 7.948374420D+05-2.318183711D+03 7.032889580D+00-1.245920568D-03 3.276693350D-07
-3.003771106D-11 5.853192770D-16                 6.957627290D+03-1.273502660D+01
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InBr2              Gurvich,1996a pt1 p292 pt2 p234.
 2 tpis96 IN  1.00BR  2.00     0.00     0.00     0.00 0  274.6260000     -149729.059
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14424.341
-6.619878900D+01-2.365897310D+02 7.926545160D+00-1.994547959D-03 2.420414153D-06
-1.548924922D-09 4.058148390D-13                 -1.895355588D+04-5.338867540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14424.341
-3.217162030D+05 4.792682100D+02 7.102649480D+00-5.514019780D-04 3.157862421D-07
-5.511254510D-11 3.172161390D-15                 -2.370923659D+04 1.193263347D-01
InBr3              Gurvich,1996a pt1 p292 pt2 p236.
 2 tpis96 IN  1.00BR  3.00     0.00     0.00     0.00 0  354.5300000     -256587.267
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19912.733
-4.990115300D+03-2.805930452D+02 1.110356060D+01-2.379995808D-03 2.887825281D-06
-1.844500707D-09 4.814395870D-13                 -3.250504910D+04-1.871748987D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19912.733
-3.505783100D+04-4.858721320D+00 1.000406131D+01-1.767620958D-06 4.164016060D-10
-5.015528870D-14 2.415414123D-18                 -3.393179240D+04-1.229069868D+01
InCL               Gurvich,1996a pt1 p281 pt2 p225
 2 tpis96 IN  1.00CL  1.00     0.00     0.00     0.00 0  150.2710000      -72147.883
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9752.117
 6.430713030D+03-2.178267726D+02 5.418830900D+00-2.048005100D-03 2.702295936D-06
-1.795319798D-09 4.847469090D-13                 -8.959841070D+03-1.202999253D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9752.117
-2.745751636D+05 8.940986910D+02 3.268118390D+00 9.180277780D-04-3.083262431D-07
 5.745458810D-11-3.645275750D-15                 -1.561603430D+04 1.266880374D+01
InCL2              Gurvich,1996a pt1 p283 pt2 p226.
 2 tpis96 IN  1.00CL  2.00     0.00     0.00     0.00 0  185.7240000     -201483.416
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13956.384
 9.935164870D+03-4.172101860D+02 8.588494910D+00-3.348385610D-03 3.997866640D-06
-2.525301853D-09 6.544490330D-13                 -2.426480269D+04-1.164521725D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13956.384
-3.328719840D+05 4.757691610D+02 7.105443690D+00-5.525786960D-04 3.160567738D-07
-5.514453680D-11 3.173680380D-15                 -2.995095917D+04-2.294555511D+00
InCL3              Gurvich,1996a pt1 p286 pt2 p228.
 2 tpis96 IN  1.00CL  3.00     0.00     0.00     0.00 0  221.1770000     -369693.227
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18306.773
 2.614743044D+04-8.414604560D+02 1.311784790D+01-6.435282470D-03 7.554874750D-06
-4.705078560D-09 1.204213663D-12                 -4.326469580D+04-3.500080940D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18306.773
-7.114043630D+04-1.628425068D+01 1.001309622D+01-5.544528880D-06 1.279877732D-09
-1.518261505D-13 7.226562770D-18                 -4.758974170D+04-1.669761011D+01
InF                Gurvich,1996a pt1 p272 pt2 p217.
 2 tpis96 IN  1.00F   1.00     0.00     0.00     0.00 0  133.8164032     -193419.989
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9217.111
 3.190123320D+04-5.295254260D+02 6.172886260D+00-2.986035832D-03 3.233778030D-06
-1.856975575D-09 4.465024970D-13                 -2.187176282D+04-7.591216620D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9217.111
-4.689001200D+05 1.321019051D+03 2.881329353D+00 1.041591078D-03-3.090754867D-07
 4.926646560D-11-2.699156425D-15                 -3.308369810D+04 1.396688303D+01
InF2               Gurvich,1996a pt1 p274 pt2 p218.
 2 tpis96 IN  1.00F   2.00     0.00     0.00     0.00 0  152.8148064     -457186.824
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12588.776
 7.522480210D+04-1.088616881D+03 9.481705210D+00-2.893229367D-03 1.516224649D-06
-7.989517810D-11-1.466781026D-13                 -5.124336150D+04-2.146666090D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12588.776
 4.318960340D+05-1.688472420D+03 8.925863010D+00-1.049188835D-03 2.723934190D-07
-2.882959902D-11 1.073493779D-15                 -4.673691940D+04-1.932464363D+01
InF3               Gurvich,1996a pt1 p276 pt2 p220.
 2 tpis96 IN  1.00F   3.00     0.00     0.00     0.00 0  171.8132096     -863079.566
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16320.434
 1.071608336D+05-1.660071901D+03 1.395972813D+01-5.018693260D-03 3.226367530D-06
-7.823385970D-10-3.726999800D-14                 -9.795214990D+04-4.606353470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16320.434
-1.656855506D+05-7.965889290D+01 1.005913347D+01-2.350816639D-05 5.163512930D-09
-5.888048810D-13 2.715090697D-17                 -1.068682627D+05-2.132968218D+01
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InH                Gurvich,1996a pt1 p269 pt2 p215
 2 tpis96 IN  1.00H   1.00     0.00     0.00     0.00 0  115.8259400      215016.904
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8684.104
-5.152828720D+04 7.813792590D+02-8.433385340D-01 1.044471274D-02-9.761074820D-06
 4.540635200D-09-8.169906900D-13                  2.110048908D+04 2.939346222D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8684.104
 7.797406660D+05-3.646882080D+03 9.542967350D+00-3.481281720D-03 1.304805603D-06
-2.182950701D-10 1.274009748D-14                  4.643295460D+04-3.659329230D+01
InI                Gurvich,1996a pt1 p298 pt2 p241.
 2 tpis96 IN  1.00I   1.00     0.00     0.00     0.00 0  241.7224700      26417.124
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10271.124
-4.686348740D+02-5.685530990D+01 4.781849690D+00-6.619368310D-04 1.027666742D-06
-7.270592070D-10 2.077991102D-13                  2.095570254D+03 4.885515130D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10271.124
 1.529221772D+06-4.690373680D+03 1.004593462D+01-3.140434110D-03 9.460834390D-07
-1.253862848D-10 5.949805640D-15                  3.152478143D+04-3.297697490D+01
InI2               Gurvich,1996a pt1 p300 pt2 p243.
 2 tpis96 IN  1.00I   2.00     0.00     0.00     0.00 0  368.6269400     -39460.643
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14912.757
-4.513890600D+03-1.183726870D+02 7.473110080D+00-1.034474090D-03 1.271465534D-06
-8.227820300D-10 2.178307019D-13                 -6.278536040D+03-6.667297500D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14912.757
-3.130671665D+05 4.813810700D+02 7.100914180D+00-5.506559920D-04 3.156120735D-07
-5.509170540D-11 3.171162830D-15                 -1.043012750D+04 2.141662307D+00
InI3               Gurvich,1996a pt1 p301 pt2 p245.
 2 tpis96 IN  1.00I   3.00     0.00     0.00     0.00 0  495.5314100    -105435.914
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20852.086
-8.728397170D+03-1.265914859D+02 1.050659120D+01-1.106109314D-03 1.354335766D-06
-8.709453460D-10 2.285186350D-13                 -1.508269063D+04-1.211411745D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20852.086
-2.196742567D+04-2.151167521D+00 1.000182200D+01-8.002214700D-07 1.897343164D-10
-2.296252460D-14 1.109838196D-18                 -1.572406335D+04-9.170888690D+00
InO                Gurvich,1996a pt1 p261 pt2 p212
 2 tpis96 IN  1.00O   1.00     0.00     0.00     0.00 0  130.8174000     145993.109
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9042.109
-1.154727169D+05 1.753668703D+03-6.965033810D+00 2.961698958D-02-3.123332334D-05
 1.437244720D-08-2.235519898D-12                  8.188679590D+03 6.608621260D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9042.109
-8.052130950D+05 1.693064203D+03 4.760863580D+00-7.340718400D-04 3.229597760D-07
-4.580150380D-11 1.954611725D-15                  4.005519810D+03 3.500742460D+00
InOH               Gurvich,1996a pt1 p271 pt2 p216.
 2 tpis96 IN  1.00O   1.00H   1.00     0.00     0.00 0  131.8253400    -124447.344
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10736.839
 6.123463020D+04-1.195863129D+03 1.041427981D+01-6.870002500D-03 6.214128780D-06
-2.408203181D-09 3.177641780D-13                 -1.079852170D+04-3.189890840D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10736.839
 8.525128930D+05-2.350317172D+03 7.984515140D+00 9.915815620D-05-6.212385450D-08
 1.016169575D-11-5.682557640D-16                 -1.536213610D+03-2.043107643D+01
In2Br2             Gurvich,1996a pt1 p294 pt2 p237.
 2 tpis96 IN  2.00BR  2.00     0.00     0.00     0.00 0  389.4440000    -196305.215
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21434.943
-9.221188300D+03-3.616677030D+01 1.014728771D+01-3.255775200D-04 4.022327480D-07
-2.604080237D-10 6.867689550D-14                 -2.644883479D+04-1.000360073D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21434.943
-1.290781804D+04-6.075401240D-01 1.000052163D+01-2.312058331D-07 5.517315720D-11
-6.708620190D-15 3.253841650D-19                 -2.663136878D+04-9.149949470D+00
In2Br4             Gurvich,1996a pt1 p295 pt2 p238.
 2 tpis96 IN  2.00BR  4.00     0.00     0.00     0.00 0  549.2520000    -436508.683
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31798.117
-1.425555379D+04-2.866009341D+02 1.713866292D+01-2.473506655D-03 3.017273071D-06
-1.934900430D-09 5.065874250D-13                 -5.593753060D+04-3.837105980D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31798.117
-4.453463710D+04-4.911523980D+00 1.600413764D+01-1.810579975D-06 4.281715740D-10
-5.171998020D-14 2.496142837D-18                 -5.739175410D+04-3.174906390D+01
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In2Br6            Gurvich,1996a pt1 p296 pt2 p239.
 2 tpis96 IN  2.00BR  6.00    0.00    0.00    0.00 0  709.0600000    -628683.430
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         43096.728
-1.758940752D+04-4.859034480D+02 2.391654505D+01-4.142061490D-03 5.033849320D-06
-3.219103650D-09 8.410220070D-13                -7.988844460D+04-6.437871880D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         43096.728
-6.945039480D+04-8.402368170D+00 2.200703884D+01-3.068251799D-06 7.235965730D-10
-8.722870580D-14 4.203469910D-18                -8.235759850D+04-5.322192800D+01
In2CL2            Gurvich,1996a pt1 p287 pt2 p229.
 2 tpis96 IN  2.00CL  2.00    0.00    0.00    0.00 0  300.5420000    -232177.375
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20223.895
-1.142848747D+04-1.416015827D+02 1.056853314D+01-1.244253440D-03 1.526076784D-06
-9.826402810D-10 2.580766990D-13                -3.026327087D+04-1.565104960D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20223.895
-2.616606332D+04-2.401955489D+00 1.000203984D+01-8.975190030D-07 2.130755553D-10
-2.581140900D-14 1.248404822D-18                -3.098016735D+04-1.234946505D+01
In2CL4            Gurvich,1996a pt1 p287 pt2 p230.
 2 tpis96 IN  2.00CL  4.00    0.00    0.00    0.00 0  371.4480000    -579125.856
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29456.525
 9.814083080D+03-8.488959010D+02 1.923410360D+01-6.815674240D-03 8.129220730D-06
-5.125076850D-09 1.324324755D-12                -7.027688140D+04-5.582665695D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29456.525
-8.503771790D+04-1.552464614D+01 1.601269668D+01-5.441549870D-06 1.267594997D-09
-1.514110365D-13 7.245404540D-18                -7.461921740D+04-3.691150615D+01
In2CL6            Gurvich,1996a pt1 p288 pt2 p231.
 2 tpis96 IN  2.00CL  6.00    0.00    0.00    0.00 0  442.3540000    -882340.029
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         38423.462
 3.004663159D+04-1.585621359D+03 2.796489470D+01-1.245506052D-02 1.475341213D-05
-9.252689200D-09 2.381233885D-12                -1.048828300D+05-9.788404640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         38423.462
-1.499400484D+05-2.988680816D+01 2.202425362D+01-1.033652301D-05 2.397911922D-09
-2.855307516D-13 1.363051661D-17                -1.130110233D+05-6.293985680D+01
In2F2             Gurvich,1996a pt1 p276 pt2 p221.
 2 tpis96 IN  2.00F   2.00    0.00    0.00    0.00 0  267.6328064    -532234.300
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18039.900
 7.255717100D+03-6.448265650D+02 1.247539512D+01-5.246089620D-03 6.283616210D-06
-3.974342340D-09 1.029559356D-12                -6.384892450D+04-3.108004586D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18039.900
-6.409715440D+04-1.163740672D+01 1.000956511D+01-4.114086910D-06 9.608828320D-10
-1.150013486D-13 5.511437480D-18                -6.714277850D+04-1.661718474D+01
In2F4             Gurvich,1996a pt1 p277 pt2 p222.
 2 tpis96 IN  2.00F   4.00    0.00    0.00    0.00 0  305.6296128   -1284788.126
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24763.074
 1.225213611D+05-2.444998374D+03 2.342425457D+01-1.291427120D-02 1.308700476D-05
-7.181673930D-09 1.648386404D-12                -1.466942111D+05-8.943560050D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24763.074
-2.205977486D+05-7.822083770D+01 1.605923872D+01-2.394023240D-05 5.329582790D-09
-6.144609570D-13 2.859099598D-17                -1.595716347D+05-4.469574580D+01
In2F6             Gurvich,1996a pt1 p279 pt2 p223.
 2 tpis96 IN  2.00F   6.00    0.00    0.00    0.00 0  343.6264192   -1960000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         33567.102
 1.825490583D+05-3.552111710D+03 3.275425230D+01-1.868064635D-02 1.892443162D-05
-1.038916311D-08 2.386637271D-12                -2.239648760D+05-1.363626758D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         33567.102
-3.170966380D+05-1.167440973D+02 2.208847456D+01-3.577733930D-05 7.968959040D-09
-9.191681700D-13 4.278494150D-17                -2.426661118D+05-7.155328560D+01
In2I2             Gurvich,1996a pt1 p303 pt2 p246.
 2 tpis96 IN  2.00I   2.00    0.00    0.00    0.00 0  483.4449400    -27813.524
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22058.476
-6.681925010D+03-1.449103222D+01 1.005929122D+01-1.314921486D-04 1.628373589D-07
-1.056087811D-10 2.788963879D-14                -6.279602600D+03-7.291130980D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22058.476
-8.148157300D+03-2.444544443D-01 1.000021086D+01-9.376789250D-08 2.242988180D-11
-2.732299303D-15 1.327135699D-19                -6.352651500D+03-6.947725420D+00
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Appendix D (*continued*)

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In2I4              Gurvich,1996a pt1 p304 pt2 p247.
 2 tpis96 IN  2.00I   4.00     0.00     0.00     0.00 0  737.2538800     -199143.181
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33468.979
-1.501028064D+04-9.744797900D+01 1.639383950D+01-8.659380210D-04 1.065671801D-06
-6.879252680D-10 1.810240886D-13                 -2.830388443D+04-2.986294828D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          33468.979
-2.505699251D+04-1.642155234D+00 1.600140149D+01-6.187066280D-07 1.472308565D-10
-1.786593333D-14 8.652338780D-19                 -2.879655333D+04-2.757790375D+01
In2I6              Gurvich,1996a pt1 p305 pt2 p248.
 2 tpis96 IN  2.00I   6.00     0.00     0.00     0.00 0  991.0628200     -319720.040
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          45088.120
-2.232640607D+04-2.000786874D+02 2.280417927D+01-1.761331313D-03 2.161510393D-06
-1.392400447D-09 3.658171880D-13                 -4.412547680D+04-5.273802030D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          45088.120
-4.311905850D+04-3.390350590D+00 2.200288128D+01-1.268348706D-06 3.012121900D-10
-3.649676710D-14 1.765530622D-18                 -4.513820270D+04-4.806868370D+01
In2O               Gurvich,1996a pt1 p264 pt2 p213.
 2 tpis96 IN  2.00O   1.00     0.00     0.00     0.00 0  245.6354000      -34763.707
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12796.504
 5.065653500D+04-8.070363670D+02 8.642067270D+00-1.533035446D-03 2.866419382D-07
 4.981134970D-10-2.554320291D-13                 -1.924908459D+03-1.490718759D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12796.504
-9.232786360D+04-5.201127280D+01 7.038723620D+00-1.543821179D-05 3.399700870D-09
-3.885457100D-13 1.795125270D-17                 -6.270926800D+03-4.421820410D+00
K                  Hf:Cox,1989. Sugar,1985. Gordon 1999.
 3 g 7/97 K   1.00     0.00     0.00     0.00     0.00 0   39.0983000       89000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 9.665143930D+00-1.458059455D-01 2.500865861D+00-2.601219276D-06 4.187306580D-09
-3.439722110D-12 1.131569009D-15                  9.959493490D+03 5.035822260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-3.566422360D+06 1.085289825D+04-1.054134898D+01 8.009801350D-03-2.696681041D-06
 4.715294150D-10-2.976897350D-14                 -5.875337010D+04 9.738551240D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 9.205786590D+08-6.935300280D+05 1.911270788D+02-2.305931672D-02 1.430294866D-06
-4.409335020D-11 5.366769166D-16                  5.395082190D+06-1.622158805D+03
K+                 Sugar,1985. Gordon 1999.
 3 g 6/97 K   1.00E  -1.00     0.00     0.00     0.00 0   39.0977514      514007.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 6.107516860D+04 4.347404440D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 6.107516860D+04 4.347404440D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 2.177901245D+07-1.415076630D+04 6.248954270D+00-5.187436800D-04 3.959640680D-08
-1.584335542D-12 2.603558905D-17                  1.722753576D+05-2.781728990D+01
K-                 Hotop,1985. Gordon 1999.
 3 g 9/97 K   1.00E  1.00     0.00     0.00     0.00 0   39.0988486       34418.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.394150710D+03 4.347446530D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.394150710D+03 4.347446530D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.394150710D+03 4.347446530D+00
KALF4              Gurvich,1982 pt1 p417 pt2 p441.
 2 tpis82 K   1.00AL  1.00F    4.00     0.00     0.00 0  142.0734508   -1907856.822
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21421.391
 1.199327246D+05-2.156457352D+03 1.815348004D+01 3.115762809D-03-9.511991670D-06
 8.431756230D-09-2.615583061D-12                 -2.222545809D+05-6.823299970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21421.391
-3.435135370D+05-2.420680834D+02 1.618029250D+01-7.193817680D-05 1.585712708D-08
-1.814017733D-12 8.388391180D-17                 -2.339658121D+05-5.233898700D+01
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KBO2              Gurvich,1982 pt1 p415 pt2 p439.
 2 tpis82 K   1.00B   1.00O   2.00     0.00     0.00 0   81.9081000     -668023.297
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14090.703
 4.296308650D+04-7.209616430D+02 8.349639350D+00 2.407820401D-03-1.680003427D-07
-1.231930486D-09 5.479951640D-13                -7.868523470D+04-1.476077068D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14090.703
 8.890726600D+04-1.671432436D+03 1.117483930D+01-4.513760260D-04 9.699003460D-08
-1.090027690D-11 4.976845800D-16                -7.375336080D+04-3.274749370D+01
KBr               Gurvich,1982 pt1 p396 pt2 p423.
 2 tpis82 K   1.00BR  1.00     0.00     0.00     0.00 0  119.0023000     -179250.878
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10109.122
 9.203309190D+03-2.137880361D+02 5.588509150D+00-2.753854319D-03 4.013672610D-06
-2.856323127D-09 8.135209740D-13                -2.188387013D+04-1.707501588D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10109.122
 1.562614367D+06-4.384894780D+03 9.045464600D+00-2.045680900D-03 4.401923850D-07
-1.448178289D-11-2.273338760D-15                 5.315342010D+03-2.864647026D+01
KCN               Chase,1998 p620.
 2 j 3/66 K   1.00C   1.00N   1.00     0.00     0.00 0   65.1157000       79496.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12456.334
 1.798627669D+04-6.300558970D+02 9.988695000D+00-1.076486132D-02 1.751014980D-05
-1.265592431D-08 3.469762810D-12                 1.058025371D+04-2.594060289D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12456.334
 3.615663870D+05-1.749018011D+03 8.680702670D+00-4.402350040D-04 9.249499710D-08
-1.021916855D-11 4.604767190D-16                 1.813734856D+04-2.281619241D+01
KCL               Gurvich,1982 pt1 p393 pt2 p420.
 2 tpis82 K   1.00CL  1.00     0.00     0.00     0.00 0   74.5513000     -214574.881
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9885.119
 9.058351510D+03-2.456801212D+02 5.680696190D+00-2.900127425D-03 4.130983060D-06
-2.907340629D-09 8.223850870D-13                -2.597304884D+04-3.677976854D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9885.119
-2.122945722D+05 9.346158900D+02 2.866264958D+00 1.468386693D-03-5.834260780D-07
 1.255777709D-10-9.150148000D-15                -3.273787640D+04 1.401864636D+01
KF                Gurvich,1982 pt1 p389 pt2 p417.
 2 tpis82 K   1.00F   1.00     0.00     0.00     0.00 0   58.0967032     -328444.886
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9455.114
 1.435704906D+04-3.391848230D+02 5.727906720D+00-2.518371562D-03 3.265915640D-06
-2.210110860D-09 6.212042050D-13                -3.914254420D+04-5.810999620D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9455.114
-1.483743237D+06 4.550048040D+03-1.081464319D+00 3.503965880D-03-1.093902537D-06
 1.771028824D-10-1.029032783D-14                -6.963329810D+04 4.088635920D+01
KH                Gurvich,1982 pt1 p383 pt2 p412.
 2 tpis82 K   1.00H   1.00     0.00     0.00     0.00 0   40.1062400      125399.106
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8795.106
 2.237782150D+02 1.793554623D+02 1.130735415D+00 9.966112560D-03-1.341218171D-05
 9.034529940D-09-2.409887770D-12                 1.338250358D+04 1.552739897D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8795.106
-3.752276520D+06 1.172778444D+04-1.014137678D+01 8.854548900D-03-2.517188074D-06
 3.344072360D-10-1.701157835D-14                -6.025103300D+04 1.010304590D+02
KI                Gurvich,1982 pt1 p400 pt2 p426.
 2 tpis82 K   1.00I   1.00     0.00     0.00     0.00 0  166.0027700     -128455.877
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10244.123
-4.572811740D+02-6.331769730D+01 4.823292420D+00-7.876668320D-04 1.336737911D-06
-1.000530992D-09 3.004503956D-13                -1.650340769D+04 3.552594820D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10244.123
 3.293747780D+06-1.002824194D+04 1.629302044D+01-6.696396750D-03 2.001412089D-06
-2.677673023D-10 1.273359646D-14                 4.676348670D+04-7.859123370D+01
KLi               Gurvich,1982 pt1 p419 pt2 p444.
 2 tpis82 K   1.00LI  1.00     0.00     0.00     0.00 0   46.0393000      170702.323
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10197.123
-3.426043690D+03-1.986063081D+01 4.487607050D+00 5.249535550D-04-1.207990165D-06
 1.705161047D-09-7.879994210D-13                 1.927868247D+04 1.912285942D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10197.123
 1.211296843D+07-4.081004870D+04 5.683792120D+01-3.128695515D-02 8.975062200D-06
-1.189303691D-09 5.880129180D-14                 2.738792595D+05-3.669693600D+02
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KNO2              Gurvich,1982 pt1 p406 pt2 p431.
 2 tpis82 K   1.00N   1.00O   2.00    0.00    0.00 0   85.1038000    -192497.394
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15342.606
-7.246236930D+04 1.226722811D+03-2.258926457D+00 3.019643903D-02-3.640259950D-05
 2.219135205D-08-5.471654230D-12                -3.077268960D+04 4.537172549D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15342.606
-1.689414093D+05-8.515973150D+02 1.063209586D+01-2.523254810D-04 5.573644410D-08
-6.393185920D-12 2.964484049D-16                -2.187701436D+04-2.755200432D+01
KNO3              Gurvich,1982 pt1 p409 pt2 p433.
 2 tpis82 K   1.00N   1.00O   3.00    0.00    0.00 0  101.1032000    -315832.888
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15917.112
-2.596112303D+04 8.200606610D+02-2.886015624D+00 4.207288900D-02-5.270323090D-05
 3.308561730D-08-8.365860370D-12                -4.335054470D+04 4.603187331D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15917.112
-3.183682870D+05-1.375234449D+03 1.401587531D+01-4.040660080D-04 8.900847780D-08
-1.018771993D-11 4.715982020D-16                -3.513853220D+04-4.804256439D+01
KNa               Gurvich,1982 pt1 p420 pt2 p445.
 2 tpis82 K   1.00NA  1.00    0.00    0.00    0.00 0   62.0880700     132404.327
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10574.127
 2.542405292D+04-4.119207410D+02 6.841087950D+00-6.250481380D-03 8.861013140D-06
-4.922415350D-09 6.493212470D-13                1.652599890D+04-9.136166910D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10574.127
 6.260326620D+06-2.563593614D+04 4.373335450D+01-2.672655110D-02 8.232705790D-06
-1.128503590D-09 5.663264890D-14                1.697274909D+05-2.664117219D+02
KO                Gurvich,1982 pt1 p375 pt2 p404.
 2 tpis82 K   1.00O   1.00    0.00    0.00    0.00 0   55.0977000     64733.314
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9481.114
 1.462562908D+04-3.384765650D+02 5.716607640D+00-2.363265083D-03 2.848716276D-06
-1.739858233D-09 4.431006520D-13                8.141835380D+03-4.022101520D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9481.114
 6.960103380D+05-3.304835290D+03 1.005743444D+01-4.331112000D-03 1.747281632D-06
-3.012370548D-10 1.790827870D-14                2.604972496D+04-3.448781520D+01
KOH               Gurvich,1997.
 2 g 9/97 K   1.00O   1.00H   1.00    0.00    0.00 0   56.1056400    -232000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11674.650
 1.770684196D+04-6.153205220D+02 8.684075720D+00-3.962849510D-03 3.408650590D-06
-9.601972220D-10 8.494054970D-15                -2.677903261D+04-2.174495666D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11674.650
 8.917271950D+05-2.334179072D+03 7.972578710D+00 1.038863156D-04-6.315893470D-08
 1.027938106D-11-5.736685820D-16                -1.443696469D+04-2.076401416D+01
K2                Gurvich,1982 pt1 p370 pt2 p402.
 2 tpis82 K   2.00    0.00    0.00    0.00    0.00 0   78.1966000     126546.329
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10741.129
 1.524169293D+04-3.301789360D+02 7.070795950D+00-9.767072460D-03 2.021535863D-05
-1.886092452D-08 6.112974640D-12                1.533402849D+04-9.101035800D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10741.129
-2.734470745D+07 6.562180010D+04-4.476350440D+01 8.938859150D-03 2.984557092D-06
-1.064158914D-09 8.334936930D-14                -4.226243830D+05 3.867142510D+02
K2+               Gurvich,1982 pt1 p374 pt2 p403.
 2 tpis82 K   2.00E  -1.00    0.00    0.00    0.00 0   78.1960514     524660.731
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10861.131
 5.196036570D+04-6.113382530D+02 7.264990540D+00-5.810634820D-03 6.567496500D-06
-2.378020865D-09-1.318637581D-13                6.479820270D+04-1.042370517D+01
   1000.000   3000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10861.131
 1.107950739D+07-4.177483820D+04 6.448659840D+01-4.024998030D-02 1.360587923D-05
-2.361920107D-09 1.673430610D-13                3.177612050D+05-4.105063100D+02
K2Br2             Gurvich,1982 pt1 p397 pt2 p424.
 2 tpis82 K   2.00BR  2.00    0.00    0.00    0.00 0  238.0046000    -538744.193
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20951.806
-1.093040504D+04-4.856651480D+01 1.019754923D+01-4.363157100D-04 5.387173660D-07
-3.486116500D-10 9.190702950D-14                -6.758073240D+04-1.294944706D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20951.806
-1.589229976D+04-8.101379460D-01 1.000069442D+01-3.074491521D-07 7.331024160D-11
-8.908944780D-15 4.319245430D-19                -6.782595440D+04-1.180425726D+01
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K2CO3             Gurvich,1982 pt1 p411 pt2 p435.
 2 tpis82 K   2.00C   1.00O   3.00     0.00     0.00 0  138.2055000     -811649.163
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19515.837
-4.407406700D+04 7.069815440D+02 6.931482470D-01 3.967831320D-02-4.850958300D-05
 2.976635787D-08-7.374761530D-12                 -1.033913232D+05 2.980651689D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19515.837
-3.264263160D+05-1.521168973D+03 1.712283562D+01-4.464580710D-04 9.833379630D-08
-1.125478371D-11 5.210069120D-16                 -9.488275100D+04-6.215220630D+01
K2C2N2            Chase,1998 p678.
 2 j 3/66 K   2.00C   2.00N   2.00     0.00     0.00 0  130.2314000      -8368.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24786.242
 4.627789480D+03-9.729810620D+02 1.996665910D+01-1.953015081D-02 3.275330460D-05
-2.393985120D-08 6.596548240D-12                 -7.774411260D+02-6.755613632D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24786.242
 7.269599500D+05-3.492108680D+03 1.835676822D+01-8.785475140D-04 1.845532919D-07
-2.038717568D-11 9.185420990D-16                  1.582600773D+04-6.728484052D+01
K2CL2             Gurvich,1982 pt1 p393 pt2 p421.
 2 tpis82 K   2.00CL  2.00     0.00     0.00     0.00 0  149.1026000     -615393.663
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19963.448
-1.328526456D+04-1.241832429D+02 1.050035730D+01-1.097776004D-03 1.348871402D-06
-8.697215120D-10 2.286584080D-13                 -7.644363150D+04-1.790150052D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19963.448
-2.614611331D+04-2.096229095D+00 1.000178456D+01-7.864803710D-07 1.869281152D-10
-2.266272348D-14 1.096790704D-18                 -7.707189330D+04-1.499720802D+01
K2F2              Gurvich,1982 pt1 p389 pt2 p418.
 2 tpis82 K   2.00F   2.00     0.00     0.00     0.00 0  116.1934064      -859875.481
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18125.626
-1.611833856D+03-5.135644890D+02 1.199922511D+01-4.280109550D-03 5.165387540D-06
-3.285814900D-09 8.549648750D-13                 -1.039248602D+05-3.039925079D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18125.626
-5.740892530D+04-9.046182110D+00 1.000750685D+01-3.250764840D-06 7.630064590D-10
-9.165649530D-14 4.405048440D-18                 -1.065413546D+05-1.874037620D+01
K2I2              Gurvich,1982 pt1 p401 pt2 p427.
 2 tpis82 K   2.00I   2.00     0.00     0.00     0.00 0  332.0055400      -418915.452
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21456.548
-8.977752440D+03-2.776460169D+01 1.011331014D+01-2.508421994D-04 3.102352114D-07
-2.010096209D-10 5.304437150D-14                 -5.326208390D+04-1.032092509D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21456.548
-1.179634729D+04-4.724761550D-01 1.000040695D+01-1.807689054D-07 4.320560970D-11
-5.259699430D-15 2.553419144D-19                 -5.340210230D+04-9.664440500D+00
K2O               Gurvich,1982 pt1 p377 pt2 p407.
 2 tpis82 K   2.00O   1.00     0.00     0.00     0.00 0   94.1960000      -74086.902
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13858.298
 2.392044068D+04-5.445358390D+02 8.826403230D+00-3.481429430D-03 3.834542070D-06
-2.268494189D-09 5.569212250D-13                 -8.234291680D+03-1.663099064D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13858.298
-4.611464580D+04-1.363119524D+01 7.010530440D+00-4.323658260D-06 9.747788420D-10
-1.135283694D-13 5.325860600D-18                 -1.107222244D+04-5.768718720D+00
K2O+              Gurvich,1982 pt1 p379 pt2 p408.
 2 tpis82 K   2.00O   1.00E  -1.00     0.00     0.00 0   94.1954514      368390.321
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14138.121
 7.201102730D+03-3.336526400D+02 8.050730350D+00-1.869353797D-03 1.921291874D-06
-1.064020951D-09 2.457514799D-13                  4.389986360D+04-1.073204150D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14138.121
-3.780033500D+04-8.849537390D+00 7.006847890D+00-2.815510856D-06 6.355001500D-10
-7.408551990D-14 3.478334960D-18                  4.214519680D+04-4.418276610D+00
K2O2              Gurvich,1982 pt1 p381 pt2 p410.
 2 tpis82 K   2.00O   2.00     0.00     0.00     0.00 0  110.1954000      -191566.301
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16289.803
 4.810870610D+04-1.003601504D+03 1.154229002D+01-4.546332520D-04-1.516606209D-06
 1.799426090D-09-6.128337290D-13                 -2.057151920D+04-3.181199790D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16289.803
-1.476073073D+05-1.021932040D+02 1.007664713D+01-3.076517991D-05 6.815252810D-09
-7.828654450D-13 3.632506100D-17                 -2.592056324D+04-2.162287184D+01
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K2O2H2              Gurvich,1997.
 2 g 9/97 K   2.00O   2.00H   2.00    0.00    0.00 0  112.2112800    -641000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22384.933
 8.174788370D+03-1.130630680D+03 1.815303256D+01-7.737431080D-03 6.837614010D-06
-2.054691111D-09 7.672877510D-14                 -7.574965170D+04-6.391759470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22384.933
 1.773523196D+06-4.665292470D+03 1.694308128D+01 2.085297143D-04-1.264714762D-07
 2.057506565D-11-1.148042134D-15                 -5.051263310D+04-6.334773920D+01
K2SO4               Gurvich,1982 pt1 p404 pt2 p429.
 2 g10/99 K   2.00S   1.00O   4.00    0.00    0.00 0  174.2592000    -1095851.121
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22283.879
 6.271492310D+04-8.152049920D+02 7.455413720D+00 3.849909780D-02-5.400630980D-05
 3.654656800D-08-9.760223570D-12                 -1.304692568D+05-1.034634770D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22283.879
-5.446125640D+05-9.590667230D+02 1.971591285D+01-2.866586009D-04 6.342480640D-08
-7.281462540D-12 3.377886930D-16                 -1.337873384D+05-7.399103551D+01
Kr                  Ref-Elm. Sugar,1991.
 3 g 8/97 KR  1.00    0.00    0.00    0.00    0.00 0   83.8000000          0.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.453750000D+02 5.490956510D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.643639057D+02-7.910050820D-01 2.500920585D+00-5.328164110D-07 1.620730161D-10
-2.467898017D-14 1.478585040D-18                 -7.403488940D+02 5.484398150D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.375531087D+09 9.064030530D+05-2.403481435D+02 3.378312030D-02-2.563103877D-06
 9.969787790D-11-1.521249677D-15                 -7.111667370D+06 2.086866326D+03
Kr+                 Sugar,1991. Gordon,1999.
 3 g 7/97 KR  1.00E  -1.00    0.00    0.00    0.00 0   83.7994514    1356953.918
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-5.650402860D+03 6.930740810D+01 2.157028132D+00 8.711228930D-04-1.181609730D-06
 7.862198630D-10-1.832589387D-13                 1.621164118D+05 8.818242260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.216567015D+05 1.166167840D+03 4.869655320D-01 1.429223599D-03-3.949628610D-07
 4.982853510D-11-2.406719258D-15                 1.556002861D+05 2.059230986D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-3.319875960D+07 1.797953100D+04-7.155015940D-01 2.671088984D-04-6.196251880D-09
-4.107025960D-13 2.000619351D-17                 1.648114259D+04 3.620325750D+01
Li                  Hf:Cox,1989. Moore,1971. Gordon,1999.
 3 g 7/97 LI  1.00    0.00    0.00    0.00    0.00 0    6.9410000     159300.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.841390197D+04 2.447622965D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.125610652D+06-3.463536730D+03 6.566611920D+00-2.260983356D-03 5.922289160D-07
-6.281635100D-11 2.884948238D-15                 4.034637400D+04-2.655918195D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.604352623D+09-1.521952201D+06 3.454400500D+02-3.779674850D-02 2.222420069D-06
-6.691570800D-11 8.088023606D-16                 1.217791847D+07-3.006680193D+03
Li+                 Moore,1971. Gordon,1999.
 3 g 3/97 LI  1.00E  -1.00    0.00    0.00    0.00 0    6.9404514     685719.428
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 8.172724550D+04 1.754357228D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 8.172724550D+04 1.754357228D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 8.172724550D+04 1.754357228D+00
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Li-                Hotop,1985. Gordon,1999.
 3 g 1/98 LI  1.00E   1.00     0.00     0.00     0.00 0    6.9415486       93474.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.049698659D+04 1.754594332D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.049698659D+04 1.754594332D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.049698659D+04 1.754594332D+00
LiALF4             Gurvich,1982 pt1 p300 pt2 p333.
 2 tpis82 LI  1.00AL  1.00F   4.00     0.00     0.00 0  109.9161508   -1857287.824
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           19534.389
 1.761529360D+05-2.999300134D+03 2.079739570D+01-1.742914656D-03-4.266642090D-06
 5.362829770D-09-1.866817087D-12                -2.117947828D+05-8.762725890D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           19534.389
-4.020700930D+05-2.783355146D+02 1.620791185D+01-8.316341570D-05 1.836905690D-08
-2.104932808D-12 9.747253020D-17                -2.278696416D+05-5.597304840D+01
LiBO2              Gurvich,1982 pt1 p299 pt2 p332.
 2 tpis82 LI  1.00B   1.00O   2.00     0.00     0.00 0   49.7508000    -652352.276
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13427.724
 6.518987570D+04-1.060320845D+03 9.548049960D+00-5.469576070D-05 2.658687599D-06
-2.931603694D-09 9.663029730D-13                -7.506204110D+04-2.490883998D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13427.724
 8.554404520D+04-1.731920898D+03 1.121462090D+01-4.659162170D-04 9.999875690D-08
-1.122880592D-11 5.123529460D-16                -7.154743820D+04-3.612397290D+01
LiBr               Gurvich,1982 pt1 p285 pt2 p318.
 2 tpis82 LI  1.00BR  1.00     0.00     0.00     0.00 0   86.8450000    -151162.890
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9173.110
 3.805620470D+04-6.129614990D+02 6.577369550D+00-4.219891760D-03 5.391423370D-06
-3.693144810D-09 1.049158761D-12                -1.637487617D+04-1.128654012D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9173.110
 6.380191420D+04-2.597050764D+02 4.656768870D+00 1.022867706D-04-5.178252340D-08
 2.058203991D-11-1.942190308D-15                -1.793363752D+04-2.290806613D-01
LiCL               Gurvich,1982 pt1 p281 pt2 p314.
 2 tpis82 LI  1.00CL  1.00     0.00     0.00     0.00 0   42.3940000    -193779.891
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9060.109
 4.964399500D+04-7.187346620D+02 6.785147030D+00-4.522145460D-03 5.748483700D-06
-3.966255670D-09 1.137911398D-12                -2.091014703D+04-1.406383901D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9060.109
-2.352769705D+05 6.120046920D+02 3.634293730D+00 6.810973320D-04-2.174238799D-07
 4.220403610D-11-2.848628426D-15                -2.862358494D+04 5.618511135D+00
LiF                Gurvich,1982 pt1 p275 pt2 p310.
 2 tpis89 LI  1.00F   1.00     0.00     0.00     0.00 0   25.9394032    -340944.894
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8828.106
 2.912537320D+04-2.531413159D+02 3.539727980D+00 3.695917040D-03-4.829466150D-06
 2.944090711D-09-6.838794740D-13                -4.064849660D+04 2.325294408D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8828.106
-3.784246490D+05 7.668062460D+02 3.585473400D+00 6.031084350D-04-1.588764206D-07
 2.569397177D-11-1.406798386D-15                -4.756469450D+04 4.385163290D+00
LiH                Gurvich,1982 pt1 p265 pt2 p301.
 2 tpis82 LI  1.00H   1.00     0.00     0.00     0.00 0    7.9489400     139264.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8686.104
-4.913731570D+04 7.756092190D+02-1.011102377D+00 1.145479597D-02-1.151038734D-05
 5.875068960D-09-1.196789735D-12                 1.204858910D+04 2.568801877D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8686.104
-2.633686357D+06 6.996429170D+03-3.233533060D+00 4.033935980D-03-9.099579640D-07
 8.775909870D-11-2.889490251D-15                -2.990043016D+04 4.971984500D+01
LiI                Gurvich,1982 pt1 p289 pt2 p322.
 2 tpis82 LI  1.00I   1.00     0.00     0.00     0.00 0  133.8454700     -85269.888
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9290.112
 4.071976370D+04-6.667289470D+02 7.064257530D+00-5.480041020D-03 6.905790160D-06
-4.537168520D-09 1.226373296D-12                -8.235487020D+03-1.296236234D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9290.112
 1.616342632D+06-4.877717080D+03 9.987186550D+00-2.889137815D-03 8.037313770D-07
-9.028172610D-11 3.078321954D-15                 1.937718764D+04-3.729276310D+01
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LiN               Chase,1998 p1500.
 2 j12/66 LI  1.00N   1.00    0.00    0.00    0.00 0   20.9477000      334720.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8999.148
 3.764959200D+04-4.883457630D+02 5.187373450D+00 2.275252171D-04-1.416337564D-06
 1.450236258D-09-4.790014330D-13                 4.161915310D+04-5.952157244D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8999.148
-5.993489980D+04-4.031134550D+01 4.529624210D+00 8.744156930D-05 2.557428364D-09
-2.905751800D-13 1.336125922D-17                 3.894831130D+04-1.214952896D+00
LiNO2             Gurvich,1982 pt1 p294 pt2 p327.
 2 tpis82 LI  1.00N   1.00O   2.00    0.00    0.00 0   52.9465000     -202031.208
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13368.792
-3.133773859D+04 5.389940810D+02-2.059877081D-02 2.610777454D-02-3.209235040D-05
 1.974344044D-08-4.892199160D-12                -2.838214963D+04 2.710019529D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13368.792
-2.196671160D+05-8.610042710D+02 1.063956465D+01-2.554392587D-04 5.644478540D-08
-6.476140050D-12 3.003536591D-16                -2.313547535D+04-3.238277103D+01
LiNO3             Gurvich,1982 pt1 p296 pt2 p329.
 2 tpis82 LI  1.00N   1.00O   3.00    0.00    0.00 0   68.9459000     -311584.675
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13915.325
 1.967205518D+04 9.052795260D+01-5.109770400D-01 3.756605950D-02-4.782738650D-05
 3.029277805D-08-7.708013150D-12                -3.907563990D+04 2.746873033D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13915.325
-3.559402450D+05-1.447644737D+03 1.406684061D+01-4.236371280D-04 9.320824510D-08
-1.065894872D-11 4.930780620D-16                -3.434827460D+04-5.275382697D+01
LiO               Gurvich,1982 pt1 p256 pt2 p294.
 2 tpis82 LI  1.00O   1.00    0.00    0.00    0.00 0   22.9404000      72914.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9362.113
 3.627029760D+04-3.499363230D+02 4.394933180D+00 1.079712984D-03-8.724038810D-07
 5.607962970D-10-2.054288457D-13                 9.533330530D+03-9.058149610D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9362.113
 1.612392133D+06-5.551312340D+03 1.120573851D+01-3.437226880D-03 9.133194660D-07
-1.027902258D-10 3.822991000D-15                 4.201575470D+04-4.857354580D+01
LiOF              Chase,1998 p1069.
 2 j 9/65 LI  1.00O   1.00F   1.00    0.00    0.00 0   41.9388032     -92048.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10827.363
 5.510110690D+04-5.770688170D+02 4.424954930D+00 1.102425422D-02-1.710493381D-05
 1.234361201D-08-3.453693000D-12                -9.278986980D+03 1.238830687D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10827.363
-1.833563281D+05-2.110049301D+02 7.156818170D+00-6.249462010D-05 1.376567002D-08
-1.574099067D-12 7.277167140D-17                -1.254530277D+04-1.272130479D+01
LiOH              Gurvich,1996b.
 2 g12/96 LI  1.00O   1.00H   1.00    0.00    0.00 0   23.9483400     -229000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11336.961
 4.574190120D+03-1.030949027D+02 4.272407370D+00 8.465219230D-03-1.386148524D-05
 1.101099795D-08-3.291248210D-12                -2.848728855D+04-8.775745780D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11336.961
 8.500751370D+05-2.430540791D+03 8.055314620D+00 6.895680880D-05-5.527207460D-08
 9.368054030D-12-5.313785680D-16                -1.365894396D+04-2.457598093D+01
LiON              Chase,1998 p1501.
 2 j 9/66 LI  1.00O   1.00N   1.00    0.00    0.00 0   36.9471000     179912.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11300.979
-9.412672670D+03 1.009332300D+02 3.006187607D+00 9.890462200D-03-1.128294343D-05
 6.410291740D-09-1.466806373D-12                 1.978348318D+04 1.016334813D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11300.979
-9.740629140D+04-5.111560940D+02 7.378493870D+00-1.508777884D-04 3.329914980D-08
-3.817514290D-12 1.769558455D-16                 2.211006635D+04-1.454105040D+01
Li2               Chase,1998 p1505.
 2 j12/83 LI  2.00    0.00    0.00    0.00    0.00 0   13.8820000     215900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9675.116
 6.778481580D+03-2.246205832D+02 5.296037440D+00-1.272412017D-03 1.205843729D-06
-9.818544590D-11-2.416702607D-13                 2.573638186D+04-6.869257580D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9675.116
 3.767645400D+07-1.185747185D+05 1.482167789D+02-8.378532110D-02 2.424919798D-05
-3.275820240D-09 1.652000081D-13                 7.723072010D+05-1.021697298D+03
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Li2+              Gurvich,1982 pt1 p249 pt2 p292.
 2 tpis82 LI  2.00E  -1.00     0.00     0.00     0.00 0   13.8814514      721611.420
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9989.120
-1.040056453D+04 2.675405642D+01 4.247271750D+00 1.057450777D-03-1.281715096D-06
 1.067477239D-09-2.759413508D-13                 8.529811310D+04 5.298189960D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9989.120
 1.279931073D+07-3.492861390D+04 3.844785360D+01-1.380635397D-02 2.531394250D-06
-2.197815991D-10 7.087669250D-15                 3.117964450D+05-2.509543641D+02
Li2Br2            Gurvich,1982 pt1 p286 pt2 p319.
 2 tpis82 LI  2.00BR  2.00     0.00     0.00     0.00 0  173.6900000     -495833.524
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16950.476
 2.786312863D+04-1.005641437D+03 1.370963066D+01-7.633663300D-03 8.942905920D-06
-5.561135090D-09 1.421736784D-12                -5.762845840D+04-4.121843760D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16950.476
-8.900983360D+04-1.988916335D+01 1.001596418D+01-6.749134050D-06 1.556299963D-09
-1.844693069D-13 8.774879920D-18                -6.279989960D+04-1.943063525D+01
Li2CL2            Gurvich,1982 pt1 p282 pt2 p315.
 2 tpis82 LI  2.00CL  2.00     0.00     0.00     0.00 0   84.7880000     -597538.789
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15906.322
 5.313398610D+04-1.427266759D+03 1.512410161D+01-1.032824906D-02 1.190773317D-05
-7.312991160D-09 1.851289430D-12                -6.769860400D+04-5.285131549D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15906.322
-1.179571272D+05-3.027126342D+01 1.002397711D+01-1.003660907D-05 2.297007564D-09
-2.706930258D-13 1.281817017D-17                -7.506822590D+04-2.264970230D+01
Li2F2             Gurvich,1982 pt1 p276 pt2 p311.
 2 tpis82 LI  2.00F   2.00     0.00     0.00     0.00 0   51.8788064     -935323.076
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13766.030
 1.443166185D+05-2.466874678D+03 1.702863290D+01-1.145541210D-02 1.086098792D-05
-5.569754280D-09 1.193819664D-12                -1.026070133D+05-7.000386610D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13766.030
-2.188931683D+05-9.259814530D+01 1.006970757D+01-2.803632163D-05 6.217549520D-09
-7.146267020D-13 3.316857300D-17                -1.156611527D+05-2.729853181D+01
Li2I2             Gurvich,1982 pt1 p290 pt2 p323.
 2 tpis82 LI  2.00I   2.00     0.00     0.00     0.00 0  267.6909400     -362801.349
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17658.652
 1.014872266D+04-7.120421010D+02 1.270392960D+01-5.685536810D-03 6.770340380D-06
-4.263304890D-09 1.100658186D-12                -4.313063860D+04-3.303950980D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17658.652
-6.973587060D+04-1.316825508D+01 1.001074855D+01-4.600203780D-06 1.070510527D-09
-1.277717768D-13 6.110612240D-18                -4.677470050D+04-1.721894034D+01
Li2O              Gurvich,1982 pt1 p259 pt2 p296.
 2 tpis82 LI  2.00O   1.00     0.00     0.00     0.00 0   29.8814000     -167338.920
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12792.080
 2.636601597D+04-1.798629279D+02 4.051115220D+00 1.189981375D-02-1.730095793D-05
 1.205584550D-08-3.292733880D-12                -2.061907963D+04 1.605995610D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12792.080
 7.261487040D+05-9.543783720D+03 2.887491643D+01-1.959494099D-02 8.086339840D-06
-1.370211764D-09 8.111727190D-14                 2.990726399D+04-1.564517822D+02
Li2O+             Gurvich,1982 pt1 p260 pt2 p297.
 2 tpis82 LI  2.00O   1.00E  -1.00     0.00     0.00 0   29.8808514      439095.089
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13028.689
 1.081044623D+05-1.261961355D+03 9.692011290D+00-1.793477428D-03 3.380326900D-07
 4.143395150D-10-1.990530222D-13                 5.754976040D+04-2.915719946D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13028.689
-1.302166086D+05-1.466759528D+02 7.610729450D+00-4.469426690D-05 9.947160640D-09
-1.147038806D-12 5.339241470D-17                 5.098762310D+04-1.528011047D+01
Li2O2             Gurvich,1982 pt1 p262 pt2 p299.
 2 tpis82 LI  2.00O   2.00     0.00     0.00     0.00 0   45.8808000     -279397.988
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13548.012
 1.392619730D+05-1.764036747D+03 1.029649198D+01 7.605949950D-03-1.538519312D-05
 1.238199941D-08-3.685431570D-12                -2.638056746D+04-3.437710560D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13548.012
-2.939232153D+05-2.359107937D+02 1.017463402D+01-6.931624360D-05 1.521202834D-08
-1.733841909D-12 7.993154620D-17                -3.618481910D+04-2.904221044D+01
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Li2O2H2           Gurvich,1996b.
 2 g12/96 LI  2.00O   2.00H   2.00    0.00    0.00 0   47.8966800    -737000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15579.040
 1.894413579D+05-2.779117524D+03 1.530234911D+01 1.070738317D-02-2.510075145D-05
 2.224910575D-08-6.949359580D-12                -7.702776920D+04-6.514116940D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15579.040
 1.215377492D+06-3.982057440D+03 1.585877373D+01 7.509145680D-04-2.585218184D-07
 3.646841700D-11-1.904139406D-15                -6.738748380D+04-6.647208400D+01
Li2SO4            Chase,1998 p1522.
 2 j12/78 LI  2.00S   1.00O   4.00    0.00    0.00 0  109.9446000   -1041816.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19652.538
 1.006318702D+05-1.543457217D+03 9.670054910D+00 3.390757380D-02-4.823483810D-05
 3.267368920D-08-8.702518510D-12                -1.201939538D+05-2.911716635D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19652.538
-6.038750870D+05-1.064550976D+03 1.979557349D+01-3.188978250D-04 7.062411120D-08
-8.114439070D-12 3.766830210D-16                -1.268908595D+05-8.014316674D+01
Li3+              Gurvich,1982 pt1 p251 pt2 p293.
 2 tpis82 LI  3.00E  -1.00    0.00    0.00    0.00 0   20.8224514     756590.836
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13289.409
-6.873222290D+03-2.820780467D+02 7.922697480D+00-1.687949474D-03 1.771718993D-06
-9.972535400D-10 2.332934849D-13                9.027963650D+04-1.619319856D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13289.409
-4.355098060D+04-6.056432750D+00 7.004722890D+00-1.953320933D-06 4.429152230D-10
-5.181983190D-14 2.439894871D-18                8.879902870D+04-1.066880792D+01
Li3Br3            Gurvich,1982 pt1 p287 pt2 p320.
 2 tpis82 LI  3.00BR  3.00    0.00    0.00    0.00 0  260.5350000    -824639.193
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26036.807
 6.431966250D+04-1.823743601D+03 2.243492856D+01-1.279418260D-02 1.459200355D-05
-8.884688150D-09 2.233708050D-12                -9.480677670D+04-8.206864420D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26036.807
-1.584670201D+05-4.041360940D+01 1.603177633D+01-1.322713911D-05 3.014221791D-09
-3.540292160D-13 1.672030783D-17                -1.042470448D+05-4.405478160D+01
Li3CL3            Gurvich,1982 pt1 p283 pt2 p316.
 2 tpis82 LI  3.00CL  3.00    0.00    0.00    0.00 0  127.1820000    -976107.121
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24560.546
 9.867429000D+04-2.324074851D+03 2.378484564D+01-1.483522400D-02 1.634495612D-05
-9.675366520D-09 2.377033859D-12                -1.103839177D+05-9.474114379D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24560.546
-2.005930356D+05-5.939400190D+01 1.604590929D+01-1.885890854D-05 4.253517370D-09
-4.955560940D-13 2.325408214D-17                -1.224927071D+05-4.844413629D+01
Li3F3             Gurvich,1982 pt1 p278 pt2 p312.
 2 tpis82 LI  3.00F   3.00    0.00    0.00    0.00 0   77.8182096   -1524596.926
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20536.734
 1.823874443D+05-3.163786240D+03 2.287811928D+01-7.544903890D-03 3.446790230D-06
 2.690705228D-10-5.250840960D-13                -1.712446093D+05-9.973654990D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20536.734
-3.618664990D+05-1.937051395D+02 1.614457133D+01-5.775628500D-05 1.274057038D-08
-1.458168875D-12 6.744850030D-17                -1.882081974D+05-5.633612880D+01
Li3I3             Gurvich,1982 pt1 p290 pt2 p324.
 2 tpis82 LI  3.00I   3.00    0.00    0.00    0.00 0  401.5364100    -612457.307
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27232.694
 3.611764690D+04-1.392033487D+03 2.110791892D+01-1.046866587D-02 1.222589173D-05
-7.584135430D-09 1.935199180D-12                -7.153084580D+04-7.093882030D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27232.694
-1.266696511D+05-2.783891914D+01 1.602228068D+01-9.399364930D-06 2.163919735D-09
-2.561731922D-13 1.217394107D-17                -7.869550680D+04-4.091724060D+01
Mg                Hf:Cox,1989. Kaufman,1991a. Gordon,1999.
 3 g 6/97 MG  1.00    0.00    0.00    0.00    0.00 0   24.3050000     147100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.694658761D+04 3.634330140D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-5.364831550D+05 1.973709576D+03-3.633776900D-01 2.071795561D-03-7.738051720D-07
 1.359277788D-10-7.766898397D-15                4.829188110D+03 2.339104998D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.166012586D+09-1.008355665D+06 1.619680021D+02-8.790130350D-03-1.925690961D-08
 1.725045214D-11-4.234946112D-16                8.349525900D+06-1.469355261D+03
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Mg+                Kaufman,1991a. Gordon,1999.
 3 g 6/97 MG  1.00E  -1.00     0.00     0.00     0.00 0   24.3044514      891047.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.064223354D+05 4.327443460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-1.914758821D+04 4.877347920D+01 2.457662661D+00 1.218104674D-05 1.897261686D-09
-1.580433756D-12 2.135732238D-16                 1.061022394D+05 4.646442860D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 4.015949550D+08-2.281591735D+05 5.421745710D+01-5.983017190D-03 3.657189130D-07
-1.020737688D-11 1.024202854D-16                 1.932463961D+06-4.480157830D+02
MgBr               Gurvich,1996a pt1 p417 pt2 p331.
 2 tpis96 MG  1.00BR  1.00     0.00     0.00     0.00 0  104.2090000       6163.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9588.115
 7.361419140D+03-2.395789881D+02 5.360560420D+00-1.667141829D-03 1.981137765D-06
-1.201637202D-09 3.032148099D-13                 5.915634440D+02-1.421771179D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9588.115
 2.477604216D+04-6.417687520D+02 6.019932090D+00-1.391004302D-03 6.443330960D-07
-1.197734078D-10 7.421644240D-15                 2.824060334D+03-6.264439920D+00
MgBr2              Gurvich,1996a pt1 p420 pt2 p333.
 2 tpis96 MG  1.00BR  2.00     0.00     0.00     0.00 0  184.1130000    -306743.219
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14757.281
 2.148477999D+04-5.154528900D+02 9.273258750D+00-3.470049040D-03 3.921840790D-06
-2.377174864D-09 5.967025560D-13                -3.652443850D+04-1.791077763D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14757.281
-4.326899010D+04-1.283036001D+01 7.510024300D+00-4.152332400D-06 9.426499180D-10
-1.103873928D-13 5.201104310D-18                -3.919886020D+04-7.409168030D+00
MgCL               Gurvich,1996a pt1 p412 pt2 p328.
 2 tpis96 MG  1.00CL  1.00     0.00     0.00     0.00 0   59.7580000     -54704.887
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9363.113
 2.043995280D+04-4.072155160D+02 5.880372300D+00-2.594175042D-03 2.945953528D-06
-1.750648628D-09 4.337959330D-13                -5.851444950D+03-6.023545750D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9363.113
 1.041328453D+06-3.380158330D+03 8.637775470D+00-2.447789643D-03 7.841969440D-07
-1.126409380D-10 5.810620730D-15                 1.327188977D+04-2.703802395D+01
MgCL+              Chase,1998 p786 6/68.
 3 g 1/01 MG  1.00CL  1.00E  -1.00     0.00     0.00 0   59.7574514      646339.332
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9515.732
 8.182385120D+03-2.622253760D+02 5.419863430D+00-1.774129606D-03 2.185811127D-06
-1.418143432D-09 3.918898580D-13                 7.770403710D+04-3.780938840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9515.732
-1.268391921D+07 3.478824540D+04-3.004222950D+01 1.481739497D-02-2.470965605D-06
 1.424433718D-10 2.789613105D-16                -1.487013740D+05 2.552015117D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9515.732
 1.382463416D+08-6.324735630D+04 2.090164490D+01-1.924320270D-03 1.303442285D-07
-4.354246510D-12 5.852012920D-17                 5.856144100D+05-1.379609224D+02
MgCL2              Gurvich,1996a pt1 p416 pt2 p330.
 2 tpis96 MG  1.00CL  2.00     0.00     0.00     0.00 0   95.2110000     -399169.896
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13900.604
 3.637824680D+04-7.307844960D+02 9.661030510D+00-3.660212940D-03 3.610819350D-06
-1.928769286D-09 4.309912350D-13                -4.646914570D+04-2.360112274D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13900.604
-6.835217010D+04-2.490899393D+01 7.518783200D+00-7.564518260D-06 1.679293770D-09
-1.931706275D-13 8.971657820D-18                -5.032686910D+04-1.053268382D+01
MgF                Gurvich,1996a pt1 p408 pt2 p325.
 2 tpis96 MG  1.00F   1.00     0.00     0.00     0.00 0   43.3034032     -232266.792
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8969.108
 3.823001620D+04-4.803310390D+02 5.068468940D+00 5.212029300D-04-1.874026347D-06
 1.759241129D-09-5.609403190D-13                -2.659114296D+04-3.768969210D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8969.108
-1.695883782D+05 3.588757630D+02 3.936001650D+00 4.813044140D-04-1.658385409D-07
 3.336052290D-11-2.270104205D-15                -3.169323990D+04 4.410565900D+00
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MgF+                Chase,1998 p1071 12/75.
 3 g 2/01 MG  1.00F   1.00E  -1.00    0.00    0.00 0   43.3028546      516867.775
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8969.375
 6.413293840D+05-8.518532610D+03 4.814216910D+01-1.163071535D-01 1.622560562D-04
-1.063484590D-07 2.634809398D-11                  1.024308480D+05-2.450074295D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8969.375
-1.056852362D+07 2.077122379D+04-6.119523560D+00 2.245834831D-03-9.515738610D-08
-2.263502341D-11 2.284524246D-15                 -8.331549880D+04 8.727102380D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8969.375
 5.735804460D+07-2.157378345D+04 6.572317550D+00 1.887605214D-04-1.860864600D-08
 6.862191460D-13-8.597821080D-18                  2.477615733D+05-1.922750114D+01
MgF2                Gurvich,1996a pt1 p411 pt2 p327.
 2 tpis96 MG  1.00F   2.00    0.00    0.00    0.00 0   62.3018064     -735498.060
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12622.440
 4.338429550D+04-6.616511770D+02 7.453448520D+00 3.520814050D-03-6.955764580D-06
 5.619923480D-09-1.688028906D-12                 -8.687183670D+04-1.545476790D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12622.440
-1.244419584D+05-8.687343750D+01 7.563581230D+00-2.499267978D-05 5.440129140D-09
-6.158245760D-13 2.822792666D-17                 -9.060019440D+04-1.420796990D+01
MgF2+               Chase,1998 p1122 12/75.
 3 g 2/01 MG  1.00F   2.00E  -1.00    0.00    0.00 0   62.3012578      582692.164
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12415.064
 7.832220260D+04-1.176632752D+03 1.025829767D+01-3.755272890D-03 3.016621585D-06
-1.327098871D-09 2.465289749D-13                  7.413228550D+04-2.990883551D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12415.064
-1.502316870D+05 7.725289560D+01 7.271569360D+00 2.237529770D-04-1.003070865D-07
 1.996274309D-11-1.233278721D-15                  6.699117500D+04-1.094528006D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12415.064
 2.601903911D+07-5.388879260D+03 5.218198280D+00 7.632535320D-04-6.606231900D-08
 2.428649361D-12-3.341900910D-17                  1.228640353D+05 3.390783040D+00
MgH                 Gurvich,1996a pt1 p401 pt2 p320.
 2 tpis96 MG  1.00H   1.00    0.00    0.00    0.00 0   25.3129400      229786.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8682.104
-4.958679150D+04 7.500278650D+02-6.442047500D-01 9.826301010D-03-8.789822440D-06
 3.823353520D-09-6.003725760D-13                  2.302279383D+04 2.657165344D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8682.104
-1.005748598D+05 1.952890106D+03-1.317191549D+00 5.603665800D-03-2.137334980D-06
 3.324880500D-10-1.824672746D-14                  1.598582755D+04 3.431233160D+01
MgI                 Gurvich,1996a pt1 p420 pt2 p334.
 2 tpis96 MG  1.00I   1.00    0.00    0.00    0.00 0  151.2094700       61206.317
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9741.117
 2.943889099D+03-1.690248574D+02 5.147251830D+00-1.321186997D-03 1.623056505D-06
-1.005114222D-09 2.567337785D-13                  6.845890270D+03 8.593132250D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9741.117
-2.370562811D+06 6.916452480D+03-3.183894490D+00 4.051551140D-03-9.774290750D-07
 1.023329400D-10-3.790304870D-15                 -3.818551110D+04 5.993104380D+01
MgI2                Gurvich,1996a pt1 p423 pt2 p336.
 2 tpis96 MG  1.00I   2.00    0.00    0.00    0.00 0  278.1139400     -171706.029
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15294.471
 1.594739709D+04-4.160412720D+02 9.010638320D+00-3.090359024D-03 3.621264260D-06
-2.260138392D-09 5.809055550D-13                 -2.080441400D+04-1.412175736D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15294.471
-3.340299180D+04-9.343511780D+00 7.507468540D+00-3.147707890D-06 7.241336470D-10
-8.567664950D-14 4.069691700D-18                 -2.294555505D+04-5.241272590D+00
MgN                 Chase,1998 p1535.
 2 j 3/64 MG  1.00N   1.00    0.00    0.00    0.00 0   38.3117000      288696.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8988.881
 3.759538640D+04-4.853164280D+02 5.163054240D+00 2.591539493D-04-1.518993975D-06
 1.522840476D-09-4.992531450D-13                  3.607294610D+04-3.813908776D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8988.881
-6.018589100D+04-4.010864780D+01 4.529498950D+00 4.760490910D-05 2.547271298D-09
-2.894058118D-13 1.330639131D-17                  3.341285700D+04 7.925250209D-01
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Appendix D (*continued*)

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MgO               Gurvich,1996a pt1 p398 pt2 p318.
 3 tpis96 MG  1.00O   1.00     0.00     0.00     0.00 0   40.3044000      32261.307
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8909.107
 3.513659740D+05-5.287197160D+03 3.382060060D+01-8.400489630D-02 1.210016160D-04
-7.630795020D-08 1.701022862D-11                 2.790679519D+04-1.624886199D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8909.107
-1.586738367D+07 3.420468100D+04-1.774087677D+01 7.004963050D-03-1.104138249D-06
 8.957488530D-11-3.052513649D-15                -2.300504434D+05 1.738984472D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8909.107
 2.290059050D+06-2.073499632D+04 1.444150005D+01-1.490609900D-03 1.052119343D-07
-3.523030610D-12 4.613111760D-17                 1.490218815D+05-8.007281730D+01
MgOH              Gurvich,1996a pt1 p404 pt2 p322.
 2 tpis96 MG  1.00O   1.00H    1.00     0.00     0.00 0   41.3123400    -132428.980
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11124.284
 3.839851620D+04-7.367383640D+02 7.920664460D+00-5.950940590D-04-2.112941162D-06
 3.228282110D-09-1.214159329D-12                -1.392326188D+04-1.916078109D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11124.284
 6.648664750D+05-1.770750355D+03 7.269999270D+00 5.336842760D-04-1.980894443D-07
 3.025677088D-11-1.554849476D-15                -6.149114560D+03-1.671027009D+01
MgOH+             Chase,1998 p1285 12/75.
 3 g 1/01 MG  1.00O   1.00H   1.00E  -1.00     0.00 0   41.3117914     615769.370
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10188.370
 1.170224573D+05-1.735933343D+03 1.164059613D+01-8.449876220D-03 7.351713740D-06
-2.790223071D-09 3.514982130D-13                 8.118807670D+04-4.271174370D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10188.370
 8.296339540D+05-2.459700177D+03 8.118732020D+00 3.500579100D-05-4.670574750D-08
 8.312358260D-12-4.802836220D-16                 8.801661710D+04-2.438155217D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10188.370
-6.691779770D+06 2.437864449D+03 6.949387850D+00 6.355744850D-05-3.980850170D-09
 1.287525303D-13-1.684735436D-18                 4.948972630D+04-1.400323314D+01
Mg(OH)2           Gurvich,1996a pt1 p407 pt2 p324.
 2 tpis96 MG  1.00O   2.00H    2.00     0.00     0.00 0   58.3196800    -551995.808
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17131.558
 5.245894670D+04-1.289056383D+03 1.389327642D+01-7.806693670D-04-4.151257230D-06
 6.109473040D-09-2.274138833D-12                -6.295089150D+04-5.015353340D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17131.558
 1.713709254D+06-4.730005350D+03 1.448925967D+01 1.907819857D-04-1.226834131D-07
 2.015343753D-11-1.128993279D-15                -3.887724670D+04-5.840498120D+01
MgS               Gurvich,1996a pt1 p425 pt2 p338.
 2 tpis96 MG  1.00S   1.00     0.00     0.00     0.00 0   56.3700000     120649.311
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9234.111
-9.565788090D+03 1.443637798D+02 1.813794717D+00 1.147168775D-02-2.220170412D-05
 1.995344981D-08-6.090688740D-12                 1.276501517D+04 1.461333093D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9234.111
 2.650794328D+07-7.711355860D+04 8.463771680D+01-3.644250680D-02 8.403084420D-06
-9.539882170D-10 4.264658030D-14                 5.078931170D+05-5.834656096D+02
Mg2               Gurvich,1996a pt1 p393 pt2 p316.
 2 tpis96 MG  2.00    0.00     0.00     0.00     0.00 0   48.6100000     286513.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9542.115
 4.545195590D+03 4.115850040D+02 4.841196170D-01 4.891969650D-03-6.395536840D-06
 4.299764550D-09-1.164624418D-12                 3.181641790D+04 2.640432143D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9542.115
 3.038224994D+04 5.945240460D+01 2.352706666D+00 1.378537924D-04-5.895692040D-08
 1.104045317D-11-6.558868290D-16                 3.351036560D+04 1.588177377D+01
Mg2F4             Chase,1998 p1178.
 2 j12/75 MG  2.00F   4.00     0.00     0.00     0.00 0  124.6036128   -1718369.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21143.314
 1.511956137D+05-3.122595912D+03 2.517715088D+01-1.558723757D-02 1.552195619D-05
-8.408729050D-09 1.911618525D-12                -1.953078883D+05-1.085103537D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21143.314
-2.980610166D+05-1.201299868D+02 1.609110864D+01-3.687456290D-05 8.220317050D-09
-9.488869780D-13 4.419795330D-17                -2.117349690D+05-5.308655470D+01
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Mn                Hf:Desai,1987. Sugar,1985. Gordon,1999.
 3 g 7/97 MN  1.00    0.00    0.00    0.00    0.00 0   54.9380490     282400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.034061359D-01-1.551537349D-03 2.500009148D+00-2.723162066D-08 4.333897430D-11
-3.511093890D-14 1.136032201D-17                 3.321935190D+04 6.649325463D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 5.855155820D+03 8.838588440D+02-3.648662580D-02 2.703720687D-03-1.324971998D-06
 2.872603290D-10-1.923633570D-14                 2.867803487D+04 2.292541198D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 3.936189040D+09-2.353549748D+06 5.377244800D+02-5.824812570D-02 3.330475100D-06
-9.689631050D-11 1.133286034D-15                 1.879530161D+07-4.690097890D+03
Mn+               Sugar,1985. Gordon,1999.
 3 g 6/97 MN  1.00E  -1.00    0.00    0.00    0.00 0   54.9375004    1005871.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 3.458017700D+02-4.251151330D+00 2.521281028D+00-5.565087280D-05 8.037162210D-08
-6.093550970D-11 1.900014268D-14                 1.202533602D+05 6.683468162D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 6.471314100D+05-2.403796253D+03 5.937715750D+00-2.341014594D-03 7.464165640D-07
-9.075969730D-11 4.467879847D-15                 1.349902108D+05-1.702666341D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.717119921D+09-9.029185830D+05 1.784788847D+02-1.566770206D-02 7.346534410D-07
-1.750673350D-11 1.667889239D-16                 7.443546080D+06-1.568005804D+03
Mo                Hf:Desai,1987. Sugar,1988. Gordon,1999.
 3 g 7/97 MO  1.00    0.00    0.00    0.00    0.00 0   95.9400000     658500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 7.646367910D+01-1.159269043D+00 2.506929462D+00-2.099249725D-05 3.414779430D-08
-2.841269591D-11 9.492443321D-15                 7.845899800D+04 7.601835660D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 5.573271000D+06-1.662365811D+04 2.135147077D+01-1.003069377D-02 2.409784357D-06
-1.811267352D-10 1.034189087D-15                 1.842646473D+05-1.275326434D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 6.205038910D+09-3.855961600D+06 9.371595060D+02-1.108164544D-01 6.929123900D-06
-2.199865715D-10 2.798315513D-15                 3.062163602D+07-8.122811340D+03
Mo+               Sugar,1988. Gordon,1999.
 3 g 7/97 MO  1.00E  -1.00    0.00    0.00    0.00 0   95.9394514    1349012.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.298236623D+02-1.560279908D+00 2.507600281D+00-1.923789063D-05 2.673316651D-08
-1.937174292D-11 5.729735412D-15                 1.615103759D+05 7.442543460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.298891120D+07-3.948276230D+04 4.866599780D+01-2.605352326D-02 7.215431920D-06
-8.719164960D-10 3.788423040D-14                 4.118948570D+05-3.216791030D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.731253943D+09 8.776685240D+05-1.669716753D+02 1.732439603D-02-9.372726850D-07
 2.593422324D-11-2.913787941D-16                -6.989098130D+06 1.517101780D+03
Mo-               Hotop,1985. Gordon,1999.
 3 g10/97 MO  1.00E   1.00    0.00    0.00    0.00 0   95.9405486     580324.628
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 6.905123690D+04 7.485659540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 6.905123690D+04 7.485659540D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 6.905123690D+04 7.485659540D+00
MoO               Gurvich,1982 pt1 p25 pt2 p30.
 3 tpis89 MO  1.00O   1.00    0.00    0.00    0.00 0  111.9394000     358005.323
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10253.123
-2.801152706D+04 5.139883480D+02 1.075385931D+00 8.681048470D-03-1.111118984D-05
 7.234349330D-09-1.893138381D-12                 3.941374080D+04 2.272230239D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10253.123
 1.573131992D+06-5.241483580D+03 1.102656868D+01-3.902996620D-03 1.147334134D-06
-1.358975691D-10 5.775268580D-15                 7.448972000D+04-4.253612930D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10253.123
 2.846838911D+08-1.710122789D+05 4.036556200D+01-2.750495204D-03 8.916821240D-08
-1.248340135D-12 3.675821910D-18                 1.408558917D+06-3.171602770D+02
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MoO2              Gurvich,1982 pt1 p28 pt2 p33.
 2 tpis82 MO  1.00O   2.00    0.00    0.00    0.00 0  127.9388000     -15558.079
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10707.025
 3.247183220D+04-1.904783783D+02 2.120771647D+00 1.650280086D-02-2.381696822D-05
 1.652371586D-08-4.494452430D-12                -1.862932837D+03 1.640582056D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10707.025
 3.096143654D+05-1.932750274D+03 9.428673180D+00-1.630508855D-03 5.752760170D-07
-7.590457470D-11 3.461337780D-15                 7.327725180D+03-2.533315948D+01
MoO3              Gurvich,1982 pt1 p31 pt2 p35.
 2 tpis82 MO  1.00O   3.00    0.00    0.00    0.00 0  143.9382000     -364412.371
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13192.785
 5.977385360D+04-7.684557830D+02 5.881844440D+00 1.686119817D-02-2.582485043D-05
 1.850382718D-08-5.152249850D-12                -4.155872390D+04-6.529162160D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13192.785
-4.097597270D+05 2.379066513D+02 9.311100800D+00 6.579338910D-04-2.895307725D-07
 5.692637260D-11-3.489657310D-15                -4.923738720D+04-2.114864892D+01
MoO3-             Gurvich,1982 pt1 p32 pt2 p36.
 2 tpis82 MO  1.00O   3.00E   1.00    0.00    0.00 0  143.9387486     -655242.501
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13560.083
 1.821617352D+05-2.224656970D+03 1.320405967D+01-1.249800352D-03-1.864166983D-06
 2.276579470D-09-7.366564570D-13                -6.938986000D+04-4.699377210D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13560.083
-4.881098720D+05 1.848536991D+01 1.042644941D+01-6.265557910D-04 3.020554347D-07
-4.733195890D-11 2.527517727D-15                -8.337815500D+04-2.701522825D+01
Mo2O6             Gurvich,1982 pt1 p33 pt2 p37.
 2 tpis82 MO  2.00O   6.00    0.00    0.00    0.00 0  287.8764000    -1149446.813
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25763.499
 1.568375811D+05-2.159930184D+03 1.522500503D+01 3.194198900D-02-5.063877150D-05
 3.689371820D-08-1.037872908D-11                -1.309931161D+05-5.408918500D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25763.499
-6.312238160D+05-6.642827550D+02 2.249383570D+01-1.968470329D-04 4.336740610D-08
-4.959777990D-12 2.293212733D-16                -1.430573250D+05-8.669628540D+01
Mo3O9             Gurvich,1982 pt1 p34 pt2 p38.
 2 tpis82 MO  3.00O   9.00    0.00    0.00    0.00 0  431.8146000    -1902031.349
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         40784.119
 1.483386187D+05-1.863895133D+03 1.738405871D+01 6.233012320D-02-9.328441350D-05
 6.613638790D-08-1.830607518D-11                -2.248945631D+05-5.826669470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         40784.119
-9.230290540D+05-1.076171759D+03 3.480007260D+01-3.189633800D-04 7.028397040D-08
-8.039642640D-12 3.717879530D-16                -2.357422166D+05-1.448769485D+02
Mo4O12            Gurvich,1982 pt1 p36 pt2 p39.
 2 tpis82 MO  4.00O  12.00    0.00    0.00    0.00 0  575.7528000    -2625526.773
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         54893.850
 2.234876437D+05-2.996203728D+03 2.682458827D+01 7.597345720D-02-1.155247012D-04
 8.256472570D-08-2.296764551D-11                -3.084619476D+05-1.065236386D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         54893.850
-1.225283388D+06-1.368141197D+03 4.701687810D+01-4.052910200D-04 8.928472390D-08
-1.021091158D-11 4.721091690D-16                -3.256477770D+05-2.047486535D+02
Mo5O15            Gurvich,1982 pt1 p38 pt2 p40.
 2 tpis82 MO  5.00O  15.00    0.00    0.00    0.00 0  719.6910000    -3329108.437
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         68917.342
 2.768903251D+05-3.757933100D+03 3.408197760D+01 9.485414960D-02-1.442672100D-04
 1.031163900D-07-2.868600013D-11                -3.913507030D+05-1.426449143D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         68917.342
-1.535389516D+06-1.710367122D+03 5.927125780D+01-5.066836290D-04 1.116223706D-07
-1.276562233D-11 5.902318910D-16                -4.128972380D+05-2.651287167D+02
N                 Hf:Cox,1989. Moore,1975. Gordon,1999.
 3 g 5/97 N   1.00    0.00    0.00    0.00    0.00 0   14.0067000     472680.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.610463780D+04 4.193905036D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 8.876501380D+04-1.071231500D+02 2.362188287D+00 2.916720081D-04-1.729515100D-07
 4.012657880D-11-2.677227571D-15                 5.697351330D+04 4.865231506D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 5.475181050D+08-3.107574980D+05 6.916782740D+01-6.847988130D-03 3.827572400D-07
-1.098367709D-11 1.277986024D-16                 2.550585618D+06-5.848769753D+02
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N+                Moore,1975. Gordon,1999.
 3 g 6/97 N   1.00E  -1.00    0.00    0.00    0.00 0   14.0061514     1882127.624
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7116.524
 5.237079210D+03 2.299958315D+00 2.487488821D+00 2.737490756D-05-3.134447576D-08
 1.850111332D-11-4.447350984D-15                 2.256284738D+05 5.076830786D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7116.524
 2.904970374D+05-8.557908610D+02 3.477389290D+00-5.288267190D-04 1.352350307D-07
-1.389834122D-11 5.046166279D-16                 2.310809984D+05-1.994146545D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7116.524
 1.646092148D+07-1.113165218D+04 4.976986640D+00-2.005393583D-04 1.022481356D-08
-2.691430863D-13 3.539931593D-18                 3.136284696D+05-1.706646380D+01
N-                Hotop,1985. Chase,1998 p1602. Gordon,1999.
 3 j12/82 N   1.00E   1.00    0.00    0.00    0.00 0   14.0072486      473537.545
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6498.345
 1.445682471D+03 7.335205110D+00 2.476680939D+00 4.227869180D-05-4.426293320D-08
 2.490985431D-11-5.831608090D-15                 5.617625000D+04 5.145753977D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6498.345
 2.404189576D+03 2.954965336D-01 2.499789368D+00 8.307564970D-08-1.829942770D-11
 2.100136461D-15-9.754986710D-20                 5.621413890D+04 5.006484157D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6498.345
 1.884379470D+03 3.905516910D-01 2.499914043D+00 9.818512540D-09-6.126037340D-13
 1.980010689D-17-2.593295116D-22                 5.621304520D+04 5.005647607D+00
NCO               Hf:East,1993. Jacox,1998 p184.
 2 g 6/01 N   1.00C   1.000   1.00    0.00    0.00 0   42.0168000      131847.241
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10198.245
 1.136503036D+04-2.444613367D+02 4.671376100D+00 2.309387548D-03 2.798649599D-06
-4.546357380D-09 1.692880931D-12                 1.577649188D+04-2.171476903D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10198.245
 1.089445289D+05-1.735459316D+03 8.655610330D+00-4.053229260D-04 7.599716410D-08
-7.253804150D-12 3.244872410D-16                 2.365792776D+04-2.619532970D+01
ND                Hf:est. from NH,H&D data. Chase,1998 p1037 6/77.
 2 g 4/01 N   1.00D   1.00    0.00    0.00    0.00 0   16.0208020      355738.797
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8648.000
 2.290155757D+04-3.957388510D+02 6.179010330D+00-8.847806970D-03 1.441582970D-05
-1.006647227D-08 2.654403586D-12                 4.355913430D+04-1.180414072D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8648.000
 5.439657960D+05-2.084583507D+03 5.834089720D+00-4.189393360D-04 9.768929530D-08
-1.056317654D-11 4.683079210D-16                 5.466633410D+04-1.480810939D+01
ND2               Hf:est. from NH2,H,&D data. Jacox,1998 p133.
 2 g 4/01 N   1.00D   2.00    0.00    0.00    0.00 0   18.0349040      184836.570
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9962.325
 1.935222164D+04-2.130631713D+02 4.844017600D+00-2.516949288D-03 7.616381540D-06
-5.464501770D-09 1.292736999D-12                 2.211998374D+04-3.171712417D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9962.325
 1.631308357D+06-6.564637490D+03 1.280547961D+01-3.094456779D-03 9.181660230D-07
-1.241119284D-10 6.226299860D-15                 6.108929580D+04-6.124502693D+01
ND3               Hf:est. from NH3,H,&D data. Chase,1998 p1047 6/77.
 2 g 4/01 N   1.00D   3.00    0.00    0.00    0.00 0   20.0490060      -54752.106
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10234.000
 1.045120370D+04 1.610166943D+02 8.574963230D-01 1.319688794D-02-1.153090144D-05
 7.142495560D-09-2.109194351D-12                -8.220948900D+03 1.675921299D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10234.000
 2.599516958D+06-1.013420124D+04 1.798028169D+01-3.582609800D-03 1.009922000D-06
-1.537638609D-10 9.106175650D-15                 5.397205660D+04-9.810988569D+01
NF                Gurvich,1989 pt1 p372 pt2 p234. Gurvich,1978 pt2 p243.
 2 tpis89 N   1.00F   1.00    0.00    0.00    0.00 0   33.0051032      232990.500
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8738.105
-3.504927750D+04 6.674502990D+02-1.201665982D+00 1.452074253D-02-1.822873148D-05
 1.160136864D-08-2.973416333D-12                 2.395414002D+04 3.089260431D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8738.105
 8.002987330D+05-3.237696580D+03 8.703408870D+00-2.701025798D-03 9.150042110D-07
-1.365256630D-10 7.234624410D-15                 4.642819450D+04-3.019933248D+01
NF2               Gurvich,1989 pt1 p373. McBride,1992 METHOD NRRAO1.
 2 g 4/99 N   1.00F   2.00    0.00    0.00    0.00 0   52.0035064       34421.447
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10581.605
 1.511831104D+04 9.196389940D+01 4.947301790D-01 2.001847323D-02-2.767712684D-05
 1.872924867D-08-5.020318040D-12                 2.839279606D+03 2.270515670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10581.605
-1.945010078D+05-3.536034070D+02 7.263494360D+00-8.402380400D-05 2.326721111D-08
-2.667577562D-12 1.236070614D-16                 3.435440590D+03-1.336102511D+01
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Appendix D (*continued*)

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NF3                Gurvich,1989 pt1 p375. McBride,1992 METHOD NRRAO2.
 2 g 4/99 N   1.00F   3.00    0.00    0.00    0.00 0   71.0019096    -131700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11854.511
 8.757149280D+04-9.031832890D+02 4.027417270D+00 2.314439555D-02-3.415106470D-05
 2.409483651D-08-6.633464190D-12                -1.237232074D+04 3.026430713D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11854.511
-3.496268760D+05-4.973728670D+02 1.036866128D+01 8.900687650D-05 5.882654360D-08
-3.157737664D-12 1.714329953D-16                -1.713183352D+04-3.098920858D+01
NH                 Hf:Anderson,1989. Gurvich,1978 pt2 p223.
 3 g 4/99 N   1.00H   1.00    0.00    0.00    0.00 0   15.0146400     357032.001
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8601.103
 1.359651320D+04-1.900296604D+02 4.518496790D+00-2.432776899D-03 2.377587464D-06
-2.592797084D-10-2.659680792D-13                4.280972190D+04-3.886561616D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8601.103
 1.958141991D+06-5.782861300D+03 9.335742020D+00-2.292910311D-03 6.076092480D-07
-6.647942750D-11 2.384234783D-15                7.898912340D+04-4.116970400D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8601.103
 9.524636790D+07-8.585826910D+04 2.980445181D+01-2.979563697D-03 1.656334158D-07
-4.744791840D-12 5.570148290D-17                6.961434270D+05-2.229027419D+02
NH+                Hf:Gibson,1985. Gurvich,1989 pt2 p216.
 3 g 5/99 N   1.00H   1.00E -1.00    0.00    0.00 0   15.0140914    1665787.914
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9495.114
 4.253656850D+03-2.458222206D+02 6.708919490D+00-1.038489430D-02 1.509008623D-05
-9.580512190D-09 2.333206758D-12                2.001077797D+05-1.395057632D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9495.114
 1.405709438D+06-4.136215710D+03 7.632014480D+00-1.228325778D-03 2.721187746D-07
-2.010098289D-11 3.717190180D-17                2.258975960D+05-2.786785234D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9495.114
 2.392941759D+08-1.741658624D+05 5.107907910D+01-5.567623700D-03 3.273391600D-07
-9.797978060D-12 1.186543279D-16                1.554705305D+06-4.065968960D+02
NHF                Gurvich,1989 pt1 p386 pt2 p247.
 2 tpis89 N   1.00H   1.00F   1.00    0.00    0.00 0   34.0130432     112000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10029.728
-5.110659820D+04 9.612256430D+02-2.706446594D+00 2.036562680D-02-2.425558952D-05
 1.551553017D-08-4.058458260D-12                7.909628340D+03 4.099317124D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10029.728
 9.013902720D+05-3.463397050D+03 8.705804860D+00-4.018963410D-04 2.322774501D-08
 6.280487330D-12-6.283095690D-16                3.337065340D+04-2.900483634D+01
NHF2               Gurvich,1989 pt1 p388 pt2 p249.
 2 tpis89 N   1.00H   1.00F   2.00    0.00    0.00 0   53.0114464    -103000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10807.439
-5.626113420D+04 1.205756556D+03-6.017529420D+00 3.760027690D-02-4.619198600D-05
 2.942475570D-08-7.598732360D-12               -1.897014374D+04 5.901714907D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10807.439
 7.394278990D+05-4.004471770D+03 1.221322320D+01-6.970437730D-04 1.271073981D-07
-1.247136898D-11 5.086517590D-16                9.134195980D+03-4.867843963D+01
NH2                Hf:Anderson,1989. Gurvich,1989 pt1 p349.Jacox,1998 p133.
 2 g 3/01 N   1.00H   2.00    0.00    0.00    0.00 0   16.0225800     189134.713
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9937.867
-3.118240659D+04 4.754243390D+02 1.372395176D+00 6.306429720D-03-5.987893560D-06
 4.492752340D-09-1.414073548D-12                1.928939662D+04 1.540126885D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9937.867
 2.111053740D+06-6.880627230D+03 1.132305924D+01-1.829236741D-03 5.643890090D-07
-7.886452480D-11 4.078593450D-15                6.503778560D+04-5.359155744D+01
NH2F               Gurvich,1989 pt1 p387 pt2 p248.
 2 tpis89 N   1.00H   2.00F   1.00    0.00    0.00 0   35.0209832     -75000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10104.976
-1.092374760D+05 1.844919780D+03-7.673871600D+00 3.229533440D-02-3.388108670D-05
 1.971871550D-08-4.810205150D-12               -1.878318960D+04 6.861483739D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10104.976
 1.927205340D+06-7.500447160D+03 1.395589580D+01-1.184804420D-03 2.050678670D-07
-1.908761310D-11 7.389236210D-16                3.552927340D+04-6.731185491D+01
NH3                Gurvich,1989 pt1 p354 pt2 p219. Haar,1968.
 2 tpis89 N   1.00H   3.00    0.00    0.00    0.00 0   17.0305200     -45940.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10043.121
-7.681226150D+04 1.270951578D+03-3.893229130D+00 2.145988418D-02-2.183766703D-05
 1.317385706D-08-3.332322060D-12               -1.264886413D+04 4.366014588D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10043.121
 2.452389535D+06-8.040894240D+03 1.271346201D+01-3.980186580D-04 3.552502750D-08
 2.530923570D-12-3.322700530D-16                4.386191960D+04-6.462330602D+01
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NH2OH             Hydroxylamine. Gurvich,1989 pt1 p368 pt2 p232.
 2 tpis89 N   1.00H   3.00O   1.00     0.00     0.00 0   33.0299200      -50000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11235.778
-5.617586670D+04 1.209290057D+03-6.179599060D+00 4.053116440D-02-5.190105540D-05
 3.594544580D-08-9.933681640D-12                 -1.265888352D+04 5.727932928D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11235.778
 4.878285050D+06-1.533604636D+04 2.227239990D+01-2.514583678D-03 3.339589730D-07
-1.881744532D-11 1.918174365D-16                 8.923020710D+04-1.269053624D+02
NH4+              Gurvich,1989 pt1 p355 pt2 p220.
 2 tpis89 N   1.00H   4.00E  -1.00     0.00     0.00 0   18.0379114      644904.945
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9978.772
-2.668315752D+05 3.763020690D+03-1.571327725D+01 4.548820210D-02-4.379962120D-05
 2.464478293D-08-5.961532330D-12                 5.823284720D+04 1.112087156D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9978.772
 4.141889000D+06-1.442072042D+04 2.011893564D+01-1.971492619D-03 3.112721421D-07
-2.602979969D-11 8.894342130D-16                 1.664196236D+05-1.201535761D+02
NO                Gurvich,1978,1989 pt1 p326 pt2 p203.
 3 tpis89 N   1.00O   1.00     0.00     0.00     0.00 0   30.0061000      91271.310
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9179.110
-1.143916503D+04 1.536467592D+02 3.431468730D+00-2.668592368D-03 8.481399120D-06
-7.685111050D-09 2.386797655D-12                 9.098214410D+03 6.728725490D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9179.110
 2.239018716D+05-1.289651623D+03 5.433936030D+00-3.656034900D-04 9.880966450D-08
-1.416076856D-11 9.380184620D-16                 1.750317656D+04-8.501669090D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9179.110
-9.575303540D+08 5.912434480D+05-1.384566826D+02 1.694339403D-02-1.007351096D-06
 2.912584076D-11-3.295109350D-16                -4.677501240D+06 1.242081216D+03
NO+               Cp,S,IP(NO): Gurvich,1989 pt1 p330 pt2 p205.
 3 g 5/99 N   1.00O   1.00E  -1.00     0.00     0.00 0   30.0055514      990809.704
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8670.104
 1.398106635D+03-1.590446941D+02 5.122895400D+00-6.394388620D-03 1.123918342D-05
-7.988581260D-09 2.107383677D-12                 1.187495132D+05-4.398433810D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8670.104
 6.069876900D+05-2.278395427D+03 6.080324670D+00-6.066847580D-04 1.432002611D-07
-1.747990522D-11 8.935014060D-16                 1.322709615D+05-1.519880037D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8670.104
 2.676400347D+09-1.832948690D+06 5.099249390D+02-7.113819280D-02 5.317659880D-06
-1.963208212D-10 2.805268230D-15                 1.443308939D+07-4.324044462D+03
NOCL              Gurvich,1989 pt1 p389. McBride,1992 METHOD PANDK.
 2 g 4/99 N   1.00O   1.00CL  1.00     0.00     0.00 0   65.4591000      52698.828
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11364.488
 2.308835209D+04-5.495983840D+02 7.730463360D+00-5.073910900D-03 1.062996184D-05
-8.793249700D-09 2.648180166D-12                 7.389898390D+03-1.318393021D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11364.488
-6.133413330D+05-3.919298830D+02 9.138917220D+00-2.605664613D-03 1.295687247D-06
-2.215378352D-10 1.280394898D-14                 4.517328420D+03-2.307323335D+01
NOF               Gurvich,1989 pt1 p382. McBride,1992 METHOD NRRAO2.
 2 g 4/99 N   1.00O   1.00F   1.00     0.00     0.00 0   49.0045032      -65000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10720.271
 4.755024260D+04-7.253904170D+02 7.213996360D+00-2.532427181D-03 6.377743900D-06
-5.518305880D-09 1.681935713D-12                -5.609722520D+03-1.289663616D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10720.271
 1.889069274D+06-6.731022660D+03 1.419018767D+01-3.693124620D-03 9.938575140D-07
-1.080748188D-10 4.210354430D-15                 3.209900780D+04-6.370266962D+01
NOF3              Gurvich,1989 pt1 p385 pt2 p246.
 2 tpis89 N   1.00O   1.00F   3.00     0.00     0.00 0   87.0013096     -187000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13697.653
 1.488360135D+05-2.241049812D+03 1.302355027D+01 5.463976680D-03-8.641865250D-06
 5.913659030D-09-1.577009169D-12                -1.328342568D+04-4.877320739D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13697.653
-2.785625217D+05-1.252321663D+03 1.390824337D+01-3.566687500D-04 7.785011060D-08
-8.850411970D-12 4.075980030D-16                -2.025651446D+04-5.106881859D+01
NO2               Gurvich,1989 pt1 p332 pt2 p207.
 2 g 4/99 N   1.00O   2.00     0.00     0.00     0.00 0   46.0055000      34193.019
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10208.175
-5.642038780D+04 9.633085720D+02-2.434510974D+00 1.927760886D-02-1.874559328D-05
 9.145497730D-09-1.777647635D-12                -1.547925037D+03 4.067851210D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10208.175
 7.213001570D+05-3.832615200D+03 1.113963285D+01-2.238062246D-03 6.547723430D-07
-7.611335900D-11 3.328361050D-15                 2.502497403D+04-4.305130040D+01
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NO2-              Gurvich,1989 pt1 p334 pt2 p208.
 2 tpis89 N   1.000   2.00E   1.00     0.00     0.00 0   46.0060486     -200035.591
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10177.009
-1.282067858D+04 6.990138180D+02-2.812596273D+00 2.412894252D-02-2.831606689D-05
 1.670509365D-08-3.983330130D-12                 -2.809915579D+04 4.063271510D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10177.009
 1.325710335D+05-1.557032129D+03 8.126721920D+00-2.728626780D-04-4.707541800D-08
 2.826729008D-11-2.353985481D-15                 -1.715795217D+04-2.228576043D+01
NO2CL             Gurvich,1989 pt1 p391. McBride,1992 METHOD NRRAO1.
 2 g 4/99 N   1.000   2.00CL  1.00     0.00     0.00 0   81.4585000      12500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12204.839
 8.508370340D+03-1.805383762D+02 3.785388560D+00 1.414934934D-02-1.423946765D-05
 7.028226180D-09-1.374688214D-12                  9.156246470D+02 6.958904458D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12204.839
-1.086773327D+05-1.452231167D+03 1.105656962D+01-4.000099280D-04 9.101543040D-08
-1.036656913D-11 4.781664810D-16                  6.294267320D+03-3.521239681D+01
NO2F              Gurvich,1989 pt1 p349. McBride,1992 METHOD NRRAO1.
 2 g 4/99 N   1.000   2.00F   1.00     0.00     0.00 0   65.0039032     -109000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11346.581
 5.667856950D+04-6.538251950D+02 4.472771520D+00 1.368870672D-02-1.460533236D-05
 7.779227940D-09-1.689355106D-12                 -1.102179443D+04 3.292074310D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11346.581
-1.008577842D+05-1.704722752D+03 1.122954945D+01-4.685215970D-04 1.047692566D-07
-1.189150595D-11 5.470307120D-16                 -6.891719180D+03-3.849788492D+01
NO3               Chase,1998 p1607.
 2 j12/64 N   1.000   3.00    0.00     0.00     0.00 0   62.0049000      71128.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10958.914
 3.405398410D+04 2.266670652D+02-3.793081630D+00 4.170732700D-02-5.709913270D-05
 3.834158110D-08-1.021969284D-11                  7.088112200D+03 4.273091713D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10958.914
-3.943872710D+05-8.244263530D+02 1.061325843D+01-2.448749816D-04 5.406060320D-08
-6.195466750D-12 2.870000149D-16                  8.982011730D+03-3.444666597D+01
NO3-              Gurvich,1989 pt1 p335 pt2 p209.
 2 tpis89 N   1.000   3.00E   1.00     0.00     0.00 0   62.0054486     -310779.531
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10773.105
 9.204813610D+04-3.911171150D+02-2.354356764D-01 2.836042108D-02-3.461324080D-05
 2.081787460D-08-5.021601270D-12                 -3.576411500D+04 2.299942308D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10773.105
-3.110005758D+05-1.369087552D+03 1.101342913D+01-4.036878820D-04 8.902086470D-08
-1.019733480D-11 4.723330790D-16                 -3.364321090D+04-3.878432657D+01
NO3F              Gurvich,1989 pt1 p384 pt2 p245.
 2 tpis89 N   1.000   3.00F   1.00     0.00     0.00 0   81.0033032      15000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14444.156
 6.472832030D+04-8.213134310D+02 6.194917440D+00 1.805438628D-02-1.996693240D-05
 1.124482018D-08-2.680013077D-12                  4.206661790D+03-7.016104301D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14444.156
-3.411793300D+05-2.353908798D+03 1.628114887D+01-1.910415273D-03 4.690873560D-07
-5.686040140D-11 2.720906921D-15                  9.760583980D+03-6.558153684D+01
N2                Ref-Elm. Gurvich,1978 pt1 p280 pt2 p207.
 3 tpis78 N   2.00    0.00    0.00     0.00     0.00 0   28.0134000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8670.104
 2.210371497D+04-3.818461820D+02 6.082738360D+00-8.530914410D-03 1.384646189D-05
-9.625793620D-09 2.519705809D-12                  7.108460860D+02-1.076003744D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8670.104
 5.877124060D+05-2.239249073D+03 6.066949220D+00-6.139685500D-04 1.491806679D-07
-1.923105485D-11 1.061954386D-15                  1.283210415D+04-1.586640027D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8670.104
 8.310139160D+08-6.420733540D+05 2.020264635D+02-3.065092046D-02 2.486903333D-06
-9.705954110D-11 1.437538881D-15                  4.938707040D+06-1.672099740D+03
N2+               Gurvich,1989 pt1 p323 pt2 p200.
 3 tpis89 N   2.00E  -1.00    0.00     0.00     0.00 0   28.0128514     1509508.424
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8671.100
-3.474047470D+04 2.696222703D+02 3.164916370D+00-2.132239781D-03 6.730476400D-06
-5.637304970D-09 1.621756000D-12                  1.790004424D+05 6.832974166D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8671.100
-2.845599002D+06 7.058893030D+03-2.884886385D+00 3.068677059D-03-4.361652310D-07
 2.102514545D-11 5.411996470D-16                  1.340388483D+05 5.090897022D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8671.100
-3.712829770D+08 3.139287234D+05-9.603518050D+01 1.571193286D-02-1.175065525D-06
 4.144441230D-11-5.621893090D-16                 -2.217361867D+06 8.436270947D+02
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N2-                Chase,1998 p1623.
 3 j 9/77 N   2.00E   1.00    0.00    0.00    0.00 0   28.0139486      148183.282
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.282
-8.146227110D+04 9.063600790D+02-1.520054079D-01 6.023190840D-03-2.897138445D-06
-4.129106680D-11 3.206989770D-13                 1.218808548D+04 2.638068855D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.282
 2.169637706D+05-1.275098516D+03 5.391095700D+00-3.198907510D-04 7.311051350D-08
-8.202017370D-12 3.740044700D-16                 2.424964308D+04-9.014934294D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8674.282
 1.345850786D+06-1.060565497D+03 4.732026850D+00-5.091450050D-06 1.628212099D-09
-5.224243560D-14 6.796651250D-19                 2.394627677D+04-4.297861544D+00
NCN                Hf:Gurvich,1991 pt1 p219. Jacox,1998 p180.
 2 g 6/01 N   2.00C   1.00    0.00    0.00    0.00 0   40.0241000      500456.573
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10180.177
-5.634680700D+04 7.323804580D+02-7.821401840D-01 1.838552441D-02-1.950836491D-05
 1.035712021D-08-2.208158483D-12                 5.539789700D+04 2.905308985D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10180.177
-1.641880975D+05-7.767840750D+02 7.999981870D+00-1.659081508D-04 2.983403318D-08
-3.120157047D-12 1.992698720D-16                 6.184424480D+04-2.149108820D+01
N2D2,cis           Hf:Use NASA data for N2H2,H,&D. Chase,1998 p1044 6/77.
 2 g 6/01 N   2.00D   2.00    0.00    0.00    0.00 0   32.0416040      202857.330
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10308.037
-2.743733656D+04 7.149808830D+02-2.223247620D+00 2.088722282D-02-1.821711897D-05
 8.844079940D-09-1.918010649D-12                 2.011115649D+04 3.637100195D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10308.037
 8.798074710D+05-5.299362040D+03 1.355007485D+01-1.316635227D-03 2.755816197D-07
-3.036294387D-11 1.365324117D-15                 5.356311890D+04-6.271215875D+01
N2F2               Gurvich,1989 pt1 p377 pt2 p237.
 2 tpis89 N   2.00F   2.00    0.00    0.00    0.00 0   66.0102064      62373.546
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12868.756
 1.543893150D+04-2.183635130D+02 3.890284250D+00 1.674017740D-02-2.056393090D-05
 1.258692110D-08-3.110498290D-12                 7.052038700D+03 5.265866442D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12868.756
-1.824883860D+05-9.534029960D+02 1.069795480D+01-2.759968700D-04 6.055439700D-08
-6.911215080D-12 3.192587230D-16                 9.283466960D+03-3.246968772D+01
N2F4               Gurvich,1989 pt1 p380 pt2 p240.
 2 tpis89 N   2.00F   4.00    0.00    0.00    0.00 0  104.0070128     -22000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17811.571
 1.162914512D+05-1.538660418D+03 9.054033050D+00 2.862113563D-02-4.332286990D-05
 3.067642499D-08-8.455474110D-12                 2.865277526D+03-2.476493006D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17811.571
-5.188594710D+05-6.702256510D+02 1.650109262D+01-2.006404436D-04 4.436752510D-08
-5.089808880D-12 2.359374159D-16                -5.281488900D+03-6.040513435D+01
N2H2               Gurvich,1989 pt1 p356.Trans,cis,& 1,1 in equilibrium.
 2 g 5/99 N   2.00H   2.00    0.00    0.00    0.00 0   30.0292800      211858.756
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9996.961
-1.504005163D+05 2.346687716D+03-9.405430290D+00 3.284299800D-02-3.121920401D-05
 1.721283190D-08-4.014537220D-12                 1.319384041D+04 7.832382630D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9996.961
 6.217567870D+06-1.753952096D+04 2.022730509D+01-9.757297660D-04-4.208416740D-07
 1.117921171D-10-7.627102210D-15                 1.374152574D+05-1.199559168D+02
NH2NO2             Aminyl Nitrite. Gurvich,1989 pt1 p370 pt2 p233.
 2 tpis89 N   2.00H   2.00O   2.00    0.00    0.00 0   62.0280800      -26000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12163.853
-4.573035060D+04 1.201365987D+03-8.105984110D+00 5.402715200D-02-6.438074450D-05
 4.025097920D-08-1.025154190D-11                -9.615785160D+03 6.867353357D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12163.853
 1.654040575D+06-8.125220880D+03 2.021742772D+01-1.244291821D-03 2.122804183D-07
-1.948359653D-11 7.439351360D-16                 4.230822580D+04-1.016190179D+02
N2H4               Gurvich,1989 pt1 p360 pt2 p225.
 2 g 4/99 N   2.00H   4.00    0.00    0.00    0.00 0   32.0451600      95180.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11449.304
-1.660756354D+05 3.035416736D+03-1.736889823D+01 7.159834020D-02-8.866799300D-05
 5.798970280D-08-1.530037218D-11                -3.731927230D+03 1.190002218D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11449.304
 3.293486700D+06-1.199850628D+04 2.104406814D+01-1.399381724D-03 1.933173351D-07
-1.318016127D-11 3.166400170D-16                 8.348433700D+04-1.155751024D+02
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N2O               Gurvich,1989 pt1 p337 pt2 p210.
 2 g 4/99 N   2.00O   1.00     0.00     0.00     0.00 0   44.0128000       81600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9580.935
 4.288225970D+04-6.440118440D+02 6.034351430D+00 2.265394436D-04 3.472782850D-06
-3.627748640D-09 1.137969552D-12                 1.179405506D+04-1.003128570D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9580.935
 3.438448040D+05-2.404557558D+03 9.125636220D+00-5.401667930D-04 1.315124031D-07
-1.414215100D-11 6.381066870D-16                 2.198632638D+04-3.147805016D+01
N2O+              Chase,1998 p1625.
 2 j12/70 N   2.00O   1.00E  -1.00     0.00     0.00 0   44.0122514     1332956.507
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10623.407
-5.624147080D+04 6.696211610D+02 8.781456190D-02 1.524476027D-02-1.527290811D-05
 7.827237390D-09-1.646739623D-12                 1.557295192D+05 2.562354785D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10623.407
-2.983553254D+04-1.179455967D+03 8.300186690D+00-2.887267217D-04 5.705105010D-08
-5.958885120D-12 2.835725557D-16                 1.646021769D+05-2.287356617D+01
N2O3              Gurvich,1989 pt1 p338 pt2 p211.
 2 g 4/99 N   2.00O   3.00     0.00     0.00     0.00 0   76.0116000       86630.595
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           17120.855
-9.204444170D+04 9.295520150D+02 3.203664810D+00 1.356473078D-02-6.262966070D-06
-1.402915559D-09 1.431620930D-12                 3.313622080D+03 1.844430953D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           17120.855
 7.783881860D+05-4.483024660D+03 1.666668024D+01-2.062143878D-03 5.309541710D-07
-6.190451220D-11 2.692956658D-15                 3.360912450D+04-6.739212388D+01
N2O4              Gurvich,1989 pt1 p342 pt2 p212.
 2 tpis89 N   2.00O   4.00     0.00     0.00     0.00 0   92.0110000       11110.919
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           16741.231
-3.804751440D+04 5.612828890D+02-2.083648324D-01 3.887087820D-02-4.422412260D-05
 2.498812310D-08-5.679102380D-12                -3.310794730D+03 2.963924840D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           16741.231
-4.582843760D+05-1.604749805D+03 1.674102133D+01-5.091385080D-04 1.143634670D-07
-1.316288176D-11 5.976316620D-16                 4.306900520D+03-6.569450380D+01
N2O5              Gurvich,1989 pt1 p343 pt2 p213.
 2 g 4/99 N   2.00O   5.00     0.00     0.00     0.00 0  108.0104000       13300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           20797.425
 4.007828170D+04-8.769675120D+02 1.055932981D+01 1.394613859D-02-8.884346920D-06
 8.500431150D-10 7.791550910D-13                 3.038962037D+03-2.386831860D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           20797.425
-5.325578960D+04-3.109277389D+03 2.036088958D+01-9.959901140D-04 2.401398635D-07
-3.057161911D-11 1.495915511D-15                 1.336957281D+04-8.298623341D+01
N3                Gurvich,1989 pt1 p325 pt2 p202.
 2 tpis89 N   3.00     0.00     0.00     0.00     0.00 0   42.0201000      436000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9570.906
 3.337406790D+04-2.965683604D+02 3.314279150D+00 6.721685360D-03-4.181126390D-06
 8.618442360D-10 6.883352530D-14                 5.298840620D+04 5.312776486D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9570.906
 2.529264658D+05-2.362876591D+03 9.135267130D+00-6.212870850D-04 1.324094351D-07
-1.478989640D-11 6.721230470D-16                 6.412695390D+04-3.135825973D+01
N3H               Gurvich,1989 pt1 p362 pt2 p226.
 2 g 4/99 N   3.00H   1.00     0.00     0.00     0.00 0   43.0280400      294000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10947.183
 3.242576060D+03 6.692664890D+01 1.766142217D+00 1.487411419D-02-1.539086440D-05
 9.172303550D-09-2.337205474D-12                 3.392069700D+04 1.513752057D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10947.183
 1.170469241D+06-5.102451990D+03 1.278288910D+01-8.409487160D-04 1.592142834D-07
-1.512289051D-11 6.102906630D-16                 6.428344470D+04-5.513119108D+01
Na                Hf:Cox,1989. Martin,1981. Gordon,1999.
 3 g 8/97 NA  1.00     0.00     0.00     0.00     0.00 0   22.9897700      107500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.218382949D+04 4.244028180D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 9.525723380D+05-2.623807254D+03 5.162596620D+00-1.210218586D-03 2.306301844D-07
-1.249597843D-11 7.226771190D-16                 2.912963564D+04-1.519717061D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 1.592533392D+09-9.717836660D+05 2.238443963D+02-2.380930558D-02 1.352018117D-06
-3.936971110D-11 4.630689121D-16                 7.748677260D+06-1.939615505D+03
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Na+                Martin,1981. Gordon,1999.
 3 g 1/98 NA  1.00E  -1.00    0.00    0.00    0.00 0   22.9892214     609542.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 7.256537070D+04 3.550845080D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 7.256537070D+04 3.550845080D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 3.401202990D+04-2.137774622D+01 2.505443851D+00-7.186631690D-07 5.188796390D-11
-1.944511626D-15 2.959355125D-20                 7.273413620D+04 3.503904060D+00
Na-                Hotop,1985. Gordon,1999.
 3 g 4/97 NA  1.00E   1.00    0.00    0.00    0.00 0   22.9903186      48453.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.082199670D+03 3.550916790D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.082199670D+03 3.550916790D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.082199670D+03 3.550916790D+00
NaALF4             Gurvich,1982 pt1 p359 pt2 p393.
 2 tpis82 NA  1.00AL  1.00F   4.00    0.00    0.00 0  125.9649208   -1857841.546
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20808.667
 1.315359536D+05-2.394685695D+03 1.909539612D+01 1.044339733D-03-6.949754130D-06
 6.769098140D-09-2.176199098D-12                -2.150512366D+05-7.505102130D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20808.667
-3.571177930D+05-2.496543879D+02 1.618634511D+01-7.449049300D-05 1.644510872D-08
-1.883696066D-12 8.719877450D-17                -2.279533538D+05-5.370665140D+01
NaBO2              Gurvich,1982 pt1 p358 pt2 p392.
 2 tpis82 NA  1.00B   1.00O   2.00    0.00    0.00 0   65.7995700    -633449.330
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13682.670
 5.046867360D+04-8.699970600D+02 8.942208240D+00 1.092655824D-03 1.440608828D-06
-2.254633535D-09 8.123312850D-13                -7.378318360D+04-1.951815135D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13682.670
 8.595814050D+04-1.691902222D+03 1.118847517D+01-4.564202310D-04 9.804505160D-08
-1.101655008D-11 5.029172760D-16                -6.949292060D+04-3.416353130D+01
NaBr               Gurvich,1982 pt1 p342 pt2 p379.
 2 tpis82 NA  1.00BR  1.00    0.00    0.00    0.00 0  102.8937700    -145928.882
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9821.118
-1.466827136D+04 7.622282870D+01 3.921163470D+00 1.793780908D-03-2.457391648D-06
 1.739334522D-09-4.796701380D-13                -1.926491755D+04 6.404382860D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9821.118
 8.978513020D+05-2.697899721D+03 7.545377160D+00-1.566692184D-03 4.470392740D-07
-4.832810210D-11 1.423961300D-15                -1.750862247D+03-1.856478949D+01
NaCN               Chase,1998 p634.
 2 j 3/66 NA  1.00C   1.00N   1.00    0.00    0.00 0   49.0071700     94266.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12125.972
 2.446165410D+04-7.536019970D+02 1.044966241D+01-1.168769048D-02 1.849279385D-05
-1.319387974D-08 3.589766560D-12                 1.297820493D+04-2.988519681D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12125.972
 3.665570290D+05-1.782094358D+03 8.699622630D+00-4.463297000D-04 9.362229310D-08
-1.033071320D-11 4.650466810D-16                 2.010926347D+04-2.419276094D+01
NaCL               Gurvich,1982 pt1 p337 pt2 p375.
 2 tpis82 NA  1.00CL  1.00    0.00    0.00    0.00 0   58.4427700    -181544.884
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9615.116
 4.362378350D+04-7.583034460D+02 8.259173000D+00-9.640915140D-03 1.358854616D-05
-9.667032250D-09 2.746261290D-12                -1.950409477D+04-1.936687551D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9615.116
 3.314498760D+05-8.968315650D+02 5.277287380D+00-1.475674008D-04-1.491128988D-08
 2.465673596D-11-2.730355213D-15                -1.736277667D+04-3.998288560D+00
NaF                Gurvich,1982 pt1 p332 pt2 p371.
 2 tpis82 NA  1.00F   1.00    0.00    0.00    0.00 0   41.9881732    -295156.889
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9225.111
 3.959887440D+04-6.534626070D+02 6.941173200D+00-5.307814930D-03 6.979720660D-06
-4.820425730D-09 1.364849175D-12                -3.352940890D+04-1.403212229D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9225.111
-1.092926912D+06 3.293303640D+03 4.135919840D-01 2.634994470D-03-8.384295630D-07
 1.417053025D-10-8.600270160D-15                -5.772884630D+04 2.909489906D+01
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NaH               Gurvich,1982 pt1 p326 pt2 p366.
 2 tpis82 NA  1.00H   1.00    0.00    0.00    0.00 0   23.9977100      140835.105
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8731.105
-3.222206410D+04 6.237622010D+02-9.216277510D-01 1.360765851D-02-1.659249878D-05
 1.033284544D-08-2.589726392D-12                 1.307381654D+04 2.641418597D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8731.105
-4.756184750D+06 1.452047626D+04-1.327563485D+01 1.055828277D-02-2.990041189D-06
 3.905322880D-10-1.923931194D-14                -7.632922270D+04 1.222070060D+02
NaI               Gurvich,1982 pt1 p345 pt2 p382.
 2 tpis82 NA  1.00I   1.00    0.00    0.00    0.00 0  149.8942400      -90637.880
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9952.120
 1.228868506D+04-2.857192800D+02 5.961057000D+00-3.792532580D-03 5.566881310D-06
-4.045013680D-09 1.172998933D-12                -1.088250556D+04-3.990739920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9952.120
 2.281549408D+06-7.093156630D+03 1.304994968D+01-5.013492330D-03 1.581735155D-06
-2.285837754D-10 1.195889950D-14                 3.253893620D+04-5.640023320D+01
NaLi              Gurvich,1982 pt1 p363 pt2 p396.
 2 tpis82 NA  1.00LI  1.00    0.00    0.00    0.00 0   29.9307700      178598.320
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9993.120
-6.569992760D+03-5.253940430D+00 4.329384260D+00 1.097919189D-03-1.965726597D-06
 2.086472026D-09-8.195988110D-13                 2.016224293D+04 1.413253322D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9993.120
 1.091664860D+07-3.480010640D+04 4.614311920D+01-2.260951051D-02 5.685324370D-06
-6.458143300D-10 2.696508992D-14                 2.394431755D+05-2.961780126D+02
NaNO2             Gurvich,1982 pt1 p352 pt2 p387.
 2 g10/99 NA  1.00N   1.00O   2.00    0.00    0.00 0   68.9952700     -166292.779
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14807.221
-6.934460610D+04 1.115432670D+03-1.816284973D+00 2.916366016D-02-3.505788520D-05
 2.128602855D-08-5.226211990D-12                -2.707275053D+04 4.121853253D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14807.221
-1.765557495D+05-8.635212950D+02 1.064105940D+01-2.559465044D-04 5.654465630D-08
-6.486710320D-12 3.008171243D-16                -1.868435672D+04-2.921304474D+01
NaNO3             Gurvich,1982 pt1 p355 pt2 p389.
 2 tpis82 NA  1.00N   1.00O   3.00    0.00    0.00 0   84.9946700     -285528.711
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15401.289
-2.043852507D+04 6.917093410D+02-2.397485012D+00 4.100386430D-02-5.141702580D-05
 3.228622470D-08-8.164691600D-12                -3.906401320D+04 4.174749459D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15401.289
-3.225592190D+05-1.396782195D+03 1.403092409D+01-4.098161770D-04 9.023845720D-08
-1.032543966D-11 4.778671550D-16                -3.138889875D+04-4.959121431D+01
NaO               Gurvich,1982 pt1 p318 pt2 p358.
 2 tpis82 NA  1.00O   1.00    0.00    0.00    0.00 0   38.9891700      106505.317
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9753.117
 1.857748013D+04-3.371497320D+02 5.644560020D+00-3.136926368D-03 6.330775390D-06
-5.429462470D-09 1.687183770D-12                 1.320332678D+04-4.996131150D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9753.117
 2.569744011D+05-2.269334161D+03 9.224397620D+00-3.651269100D-03 1.446811119D-06
-2.443068386D-10 1.428508328D-14                 2.413239357D+04-2.989159486D+01
NaOH              Gurvich,1996b.
 2 g12/96 NA  1.00O   1.00H   1.00    0.00    0.00 0   39.9971100     -191000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11397.671
 3.442036740D+04-7.923218180D+02 8.997932300D+00-4.079844520D-03 3.065783937D-06
-5.119189340D-10-1.541016409D-13                -2.086951091D+04-2.510590090D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11397.671
 8.753787760D+05-2.342514649D+03 7.978469890D+00 1.016451512D-04-6.268531950D-08
 1.022715136D-11-5.713286410D-16                -9.509901710D+03-2.202310401D+01
NaOH+             Chase,1998 p1297 12/71. Jacox,1994.
 3 g 2/01 NA  1.00O   1.00H   1.00E  -1.00    0.00 0   39.9965614      683862.371
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11694.871
 2.278039363D+04-6.672194220D+02 8.921593120D+00-4.481263270D-03 3.951883920D-06
-1.173341234D-09 2.041806631D-14                 8.363382190D+04-2.258912262D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11694.871
 8.815413650D+05-2.363159755D+03 8.053203930D+00 7.271279740D-05-5.897417890D-08
 1.007487881D-11-5.474406210D-16                 9.584441650D+04-2.079484012D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11694.871
-2.839326542D+07 1.778338286D+04 2.821047612D+00 5.793749100D-04-3.328793850D-08
 9.421248450D-13-1.072317149D-17                -6.175194270D+04 2.465488033D+01
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Na2              Gurvich,1982 pt1 p314 pt2 p357.
 2 tpis82 NA  2.00    0.00    0.00    0.00    0.00 0   45.9795400     142339.125
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10403.125
 6.848628680D+03-1.530836599D+02 5.325230390D+00-1.944906088D-03 2.657477888D-06
-9.096841120D-10-2.448756730D-13                 1.649170574D+04-2.653564394D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10403.125
 1.929940758D+07-6.269280120D+04 8.267682110D+01-4.565137810D-02 1.259515667D-05
-1.560445735D-09 7.024677170D-14                 4.090820800D+05-5.509970890D+02
Na2Br2           Gurvich,1982 pt1 p342 pt2 p380.
 2 tpis82 NA  2.00BR  2.00    0.00    0.00    0.00 0  205.7875400    -480848.453
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19591.547
-1.384946731D+04-1.573241177D+02 1.063192589D+01-1.383418339D-03 1.697156537D-06
-1.092992547D-09 2.870988020D-13                -6.010391820D+04-1.861473856D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19591.547
-3.021730975D+04-2.659232780D+00 1.000225819D+01-9.935490630D-07 2.358676253D-10
-2.857194816D-14 1.381909879D-18                 -6.090039920D+04-1.494517863D+01
Na2CL2           Gurvich,1982 pt1 p338 pt2 p376.
 2 tpis82 NA  2.00CL  2.00    0.00    0.00    0.00 0  116.8855400    -564401.783
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18699.327
-1.082955250D+04-3.139528641D+02 1.124411332D+01-2.697665795D-03 3.286359480D-06
-2.105377639D-09 5.508056610D-13                -6.938675430D+04-2.511011582D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18699.327
-4.412105230D+04-5.393491280D+00 1.000453407D+01-1.981155641D-06 4.680188200D-10
-5.648940680D-14 2.724721177D-18                -7.098063410D+04-1.787230397D+01
Na2F2            Gurvich,1982 pt1 p333 pt2 p372.
 2 tpis82 NA  2.00F   2.00    0.00    0.00    0.00 0   83.9763464    -834062.776
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16682.330
 2.351580802D+04-1.000737062D+03 1.375845076D+01-7.838346980D-03 9.276288700D-06
-5.813612970D-09 1.495354820D-12                -9.835831880D+04-4.381148090D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16682.330
-9.030750690D+04-1.893938035D+01 1.001535518D+01-6.539675450D-06 1.516333603D-09
-1.804877459D-13 8.613474920D-18                -1.034896664D+05-2.178860202D+01
Na2I2            Gurvich,1982 pt1 p346 pt2 p383.
 2 tpis82 NA  2.00I   2.00    0.00    0.00    0.00 0  299.7884800    -356869.932
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20246.068
-1.305063983D+04-8.992506680D+01 1.036367976D+01-8.000070190D-04 9.848777980D-07
-6.359373120D-10 1.673774775D-13                -4.551465490D+04-1.487509548D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20246.068
-2.231236397D+04-1.515570558D+00 1.000129413D+01-5.715035380D-07 1.360287207D-10
-1.650916036D-14 7.996149680D-19                -4.596921750D+04-1.276523965D+01
Na2O             Gurvich,1982 pt1 p321 pt2 p361.
 2 tpis82 NA  2.00O   1.00    0.00    0.00    0.00 0   61.9789400    -16559.830
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14410.170
 3.901149290D+04-7.266207890D+02 9.623710780D+00-3.556418640D-03 3.470704350D-06
-1.835177736D-09 4.062134710D-13                -4.593073250D+02-2.349565832D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14410.170
-6.600525160D+04-2.569021634D+01 7.519385420D+00-7.811635240D-06 1.735015890D-09
-1.996634558D-13 9.276433550D-18                -4.297339650D+03-1.063530214D+01
Na2O+            Gurvich,1982 pt1 p322 pt2 p362.
 2 tpis82 NA  2.00O   1.00E  -1.00    0.00    0.00 0   61.9783914     520833.968
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14606.568
 2.647969755D+04-5.969062160D+02 9.294129530D+00-3.080702005D-03 3.080460653D-06
-1.669452593D-09 3.789784140D-13                 6.347310250D+04-2.025274459D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14606.568
-5.740909330D+04-1.989178143D+01 7.515295260D+00-6.258333230D-06 1.407321045D-09
-1.635833952D-13 7.662445130D-18                 6.032977470D+04-9.426526740D+00
Na2O2            Gurvich,1982 pt1 p324 pt2 p364.
 2 tpis82 NA  2.00O   2.00    0.00    0.00    0.00 0   77.9783400    -123930.345
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15565.255
 7.382458920D+04-1.355125340D+03 1.255579861D+01-2.112046045D-03 4.920353520D-08
 1.003950603D-09-4.447732070D-13                -1.058858918D+04-4.021811780D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15565.255
-1.732295239D+05-1.137561118D+02 1.008529143D+01-3.422098940D-05 7.577721890D-09
-8.701256730D-13 4.036061390D-17                -1.780300574D+04-2.386789190D+01
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Na2O2H2           Gurvich,1996b.
 2 g 8/01 NA  2.00O   2.00H   2.00     0.00     0.00 0   79.9942200     -624000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19346.141
 1.089414289D+05-2.634822704D+03 2.306608858D+01-1.689310193D-02 1.673483190D-05
-7.821166010D-09 1.475034470D-12                -6.593137330D+04-9.802987580D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19346.141
 1.675713839D+06-4.704921170D+03 1.697343934D+01 1.961487616D-04-1.236951748D-07
 2.025311778D-11-1.132991623D-15                -4.856245570D+04-6.813480980D+01
Na2SO4            Gurvich,1982 pt1 p349 pt2 p385.
 2 tpis82 NA  2.00S   1.00O   4.00     0.00     0.00 0  142.0421400    -1040132.302
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20971.698
 8.344283210D+04-1.210880769D+03 8.742353000D+00 3.600796630D-02-5.117645960D-05
 3.481569040D-08-9.321931220D-12                -1.217387045D+05-2.061505785D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20971.698
-5.754483110D+05-9.817060340D+02 1.973310397D+01-2.936395520D-04 6.498708170D-08
-7.462479400D-12 3.462491660D-16                -1.270597762D+05-7.667871596D+01
Na3CL3            Gurvich,1982 pt1 p339 pt2 p377.
 2 tpis82 NA  3.00CL  3.00     0.00     0.00     0.00 0  175.3283100     -912674.509
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          29477.157
-1.254216670D+04-5.502160460D+02 1.816110649D+01-4.656515260D-03 5.646438220D-06
-3.604760320D-09 9.405556240D-13                -1.119270172D+05-5.290104960D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          29477.157
-7.160297970D+04-9.573493810D+00 1.600799614D+01-3.478356970D-06 8.190943690D-10
-9.863210030D-14 4.749005350D-18                -1.147252948D+05-4.031342160D+01
Na3F3             Gurvich,1982 pt1 p334 pt2 p373.
 2 tpis82 NA  3.00F   3.00     0.00     0.00     0.00 0  125.9645196    -1348015.386
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25602.274
 5.247030350D+04-1.775597273D+03 2.250927609D+01-1.333033615D-02 1.555790239D-05
-9.646011460D-09 2.460254271D-12                -1.580736389D+05-8.580122370D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25602.274
-1.553995698D+05-3.551970190D+01 1.602841159D+01-1.198056094D-05 2.757248730D-09
-3.263300970D-13 1.550483212D-17                -1.672141773D+05-4.753780680D+01
Nb                Hf:Gurvich,1982. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 3/98 NB  1.00    0.00     0.00     0.00     0.00 0   92.9063800     723113.099
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8354.099
 7.889660670D+04-1.212813914D+03 1.034579819D+01-1.676630056D-02 1.979119979D-05
-1.218224409D-08 3.058098336D-12                 9.165315140D+04-3.594742850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8354.099
-1.096553196D+06 2.546650713D+03 2.236054882D+00-1.280029198D-03 8.464237990D-07
-1.486269508D-10 8.714309406D-15                 6.879124550D+04 1.398169030D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8354.099
 1.818626365D+09-1.032414940D+06 2.308238005D+02-2.445004311D-02 1.395626888D-06
-4.087233010D-11 4.826490497D-16                 8.359622560D+06-1.997797290D+03
Nb+               Moore,1971. Moore,1970a. Gordon,1999.
 3 g 7/97 NB  1.00E  -1.00     0.00     0.00     0.00 0   92.9058314    1393604.675
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8589.075
 1.314447859D+05-2.000135035D+03 1.505024212D+01-2.996583942D-02 3.729868630D-05
-2.269869569D-08 5.449089902D-12                 1.760054029D+05-6.224595520D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8589.075
-1.077639646D+06 2.159046421D+03 2.310604767D+00-5.363991760D-04 5.057915090D-07
-1.032401533D-10 6.629241280D-15                 1.517945546D+05 1.210678502D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8589.075
 1.876113970D+07-2.202847919D+04 1.427004521D+01-2.295936786D-03 2.430819459D-07
-1.116131589D-11 1.836221996D-16                 3.245415600D+05-8.494555710D+01
Nb-               Hotop,1985. Gordon,1999.
 3 g 9/97 NB  1.00E   1.00     0.00     0.00     0.00 0   92.9069286     631054.008
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8653.808
-7.220924850D+04 5.259501250D+02 3.470468390D+00-4.950505530D-03 7.401859030D-06
-5.016302070D-09 1.314100719D-12                 7.178828870D+04 5.155510070D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8653.808
 1.117458019D+05 1.340072834D+02 2.391474129D+00 4.524813430D-05-1.025345000D-08
 1.195577988D-12-5.606330450D-17                 7.473996750D+04 9.675315610D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8653.808
-1.279446680D+05 1.664265071D+02 2.463334336D+00 4.161717840D-06-2.573750764D-10
 8.239892930D-15-1.069096936D-19                 7.430433860D+04 9.186188470D+00
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NbCL5             Chase,1998 p918.
 2 j12/74 NB  1.00CL  5.00    0.00    0.00    0.00 0  270.1713800    -703330.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26343.163
 7.348277970D+04-1.919172996D+03 2.290799567D+01-1.404352774D-02 1.638106985D-05
-1.018941843D-08 2.612266639D-12                -7.974118810D+04-8.439637087D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26343.163
-1.563816638D+05-4.450521280D+01 1.603544630D+01-1.489949737D-05 3.420777920D-09
-4.041124420D-13 1.917266128D-17                -8.962815120D+04-4.374582607D+01
NbO               Gurvich,1982 pt1 p76 pt2 p78.
 3 tpis82 NB  1.00O   1.00    0.00    0.00    0.00 0  108.9057800     210988.706
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8780.106
-6.797834360D+03 2.839767438D+02 5.645708400D-01 1.134928619D-02-1.549821141D-05
 1.047624988D-08-2.762937835D-12                 2.317993893D+04 2.365708974D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8780.106
 5.532258780D+05-1.287669306D+03 4.980066040D+00 1.116014163D-04 4.031838680D-08
 1.048773710D-11-1.893595022D-15                 3.268457790D+04-1.868958549D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8780.106
 5.210846640D+07-7.508889140D+04 3.023869608D+01-2.881829240D-03 1.595446362D-07
-4.532772640D-12 5.266479160D-17                 5.788974420D+05-2.169255418D+02
NbOCL3            Barin,1989. Wagman,1982.
 2 bar 89 NB  1.00O   1.00CL  3.00    0.00    0.00 0  215.2647800    -752300.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20631.000
-1.108482359D+05 1.173066983D+02 1.165558433D+01 1.287422064D-03-1.659778281D-06
 1.102107826D-09-2.949903264D-13                -9.504023920D+04-2.386450092D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20631.000
-1.515551427D+05 5.305545230D+01 1.228915282D+01-1.527366571D-04 6.778576440D-08
-9.365170650D-12 4.670036930D-16                -9.490768120D+04-2.745263834D+01
NbO2              Gurvich,1982 pt1 p80 pt2 p81.
 2 tpis82 NB  1.00O   2.00    0.00    0.00    0.00 0  124.9051800    -201266.752
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10654.352
 1.739046582D+04 3.881029440D+01 9.024299120D-01 1.909523319D-02-2.667013583D-05
 1.813901051D-08-4.872365880D-12                -2.528518558D+04 2.289323379D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10654.352
-6.851859900D+05 9.112249320D+02 6.339199840D+00-8.230080300D-05 1.984439605D-07
-3.261171490D-11 1.602430854D-15                -3.325027320D+04-3.559556550D+00
Ne                Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 5/97 NE  1.00    0.00    0.00    0.00    0.00 0   20.1797000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 3.355322720D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 3.355322720D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-1.238252746D+07 6.958579580D+03 1.016709287D+00 1.424664555D-04-4.803933930D-09
-1.170213183D-13 8.415153652D-18                -5.663933630D+04 1.648438697D+01
Ne+               Moore,1971. Moore,1970a. Gordon,1999.
 3 g 3/97 NE  1.00E  -1.00    0.00    0.00    0.00 0   20.1791514    2086965.946
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6304.214
 7.281551480D+04-8.695697990D+02 6.108646970D+00-5.841356930D-03 5.041044170D-06
-2.293759207D-09 4.339065680D-13                2.545996890D+05-1.673449355D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6304.214
-1.112742658D+05 4.765697970D+02 2.196650531D+00 1.102593151D-04-2.287564425D-08
 2.510218183D-12-1.126646096D-16                2.472536944D+05 7.466140540D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6304.214
-5.615474110D+04 1.418980160D+02 2.475716842D+00 1.944430992D-06-6.323099200D-11
-1.313313446D-16 3.534699010D-20                2.494452217D+05 5.366882220D+00
Ni                Hf:Hultgren,1973. Litzen,1993. Gordon,1999.
 3 g 8/97 NI  1.00    0.00    0.00    0.00    0.00 0   58.6934000     430116.605
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6825.013
-3.235810550D+04 6.015264620D+02-1.079270657D+00 1.089505519D-02-1.369578748D-05
 8.317725790D-09-2.019206968D-12                4.813810810D+04 2.718829200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6825.013
-4.938262210D+05 1.092909991D+03 2.410485014D+00-1.599071827D-05-1.047414069D-08
 4.624795210D-12-4.448865218D-17                4.336072170D+04 9.677195600D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6825.013
 3.492669880D+08-1.654227575D+05 3.349869360D+01-3.527085900D-03 3.240060240D-07
-1.604177606D-11 2.935430214D-16                1.409017848D+06-2.672455567D+02
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Ni+                Sugar,1985. Gordon,1999.
 3 g 8/97 NI  1.00E  -1.00    0.00    0.00    0.00 0   58.6928514    1172594.573
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6205.773
-8.969386030D+04 1.173601500D+03-3.410620410D+00 1.390739137D-02-1.501714923D-05
 7.896337900D-09-1.648686761D-12                  1.345589500D+05 4.031495160D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6205.773
-3.961999320D+06 1.017084853D+04-6.029331290D+00 2.770858029D-03-8.902077700D-08
-5.541000580D-11 5.235342833D-15                  7.340395120D+04 7.137503100D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6205.773
 5.286662360D+07-3.719827100D+04 1.470794435D+01-1.489309517D-03 8.648712770D-08
-1.705443550D-12 5.049635419D-18                  4.253204090D+05-9.590502160D+01
Ni-                Hotop,1985. Gordon,1999.
 3 g 9/97 NI  1.00E   1.00    0.00    0.00    0.00 0   58.6939486     311764.357
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6207.157
-8.437624750D+04 1.135476552D+03-3.380615830D+00 1.423003786D-02-1.582586302D-05
 8.608840410D-09-1.875316029D-12                  3.124307590D+04 3.998061300D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6207.157
-5.433424800D+05 1.182645330D+03 2.126441240D+00 3.730455940D-05 6.953608430D-09
-1.945719381D-12 1.271571579D-16                  2.854759122D+04 1.043462235D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6207.157
 2.235741343D+06-7.539321100D+02 2.675777011D+00-2.056834268D-05 1.297167360D-09
-4.210909080D-14 5.520885950D-19                  4.359114370D+04 5.724516640D+00
NiCL               Chase,1998 p794.
 2 j 9/77 NI  1.00CL  1.00    0.00    0.00    0.00 0   94.1464000     182004.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9464.921
-2.357997085D+04 2.205491630D+02 2.714260287D+00 4.453598470D-03-2.849162229D-06
-1.691898007D-10 5.156699260D-13                  1.957229490D+04 1.423643068D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9464.921
-3.905769190D+06 9.961533990D+03-3.839432340D+00 2.767979391D-03-7.005959380D-08
-5.741403660D-11 5.307635800D-15                 -4.505397050D+04 6.769402548D+01
NiCL2              Chase,1998 p840.
 2 j 9/77 NI  1.00CL  2.00    0.00    0.00    0.00 0  129.5994000     -73931.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14206.546
 7.109976530D+04-1.218958288D+03 1.208750596D+01-8.674403140D-03 1.043608104D-05
-6.298493010D-09 1.485857653D-12                 -5.006998710D+03-3.499472036D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14206.546
 1.585889817D+05-1.161488738D+03 9.608015380D+00-9.461224510D-04 2.608172043D-07
-3.264637250D-11 1.525950893D-15                 -4.578985540D+03-2.212397347D+01
NiO                Pedley,1983 p1012 p1019.
 2 g12/00 NI  1.00O   1.00    0.00    0.00    0.00 0   74.6928000     297064.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8866.569
 2.320630462D+04-1.907136094D+02 3.190178620D+00 5.291383490D-03-8.080210430D-06
 5.839812760D-09-1.639499596D-12                  3.576711120D+04 7.841265670D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8866.569
-7.234091940D+04-8.035554270D+01 4.559221020D+00 2.305154510D-05 5.139832820D-09
-5.853474910D-13 2.697077329D-17                  3.461143850D+04 1.209414814D+00
NiS                Chase,1998 p1707.
 2 j12/76 NI  1.00S   1.00    0.00    0.00    0.00 0   90.7584000     357419.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9218.527
-1.272488974D+04 1.432801381D+02 2.471951556D+00 5.505271120D-03-3.418355280D-06
-3.099052241D-10 6.268154670D-13                  4.117716080D+04 1.517981835D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9218.527
-7.358128980D+05 1.178231095D+03 4.837865580D+00-3.931201390D-04 1.341974852D-07
-1.569591708D-11 6.677045060D-16                  3.275565940D+04 3.690652283D+00
O                  D0(O2):Brix,1954. Moore,1976. Gordon,1999.
 3 g 5/97 O   1.00    0.00    0.00    0.00    0.00 0   15.9994000     249175.003
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6725.403
-7.953611300D+03 1.607177787D+02 1.966226438D+00 1.013670310D-03-1.110415423D-06
 6.517507500D-10-1.584779251D-13                  2.840362437D+04 8.404241820D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6725.403
 2.619020262D+05-7.298722030D+02 3.317177270D+00-4.281334360D-04 1.036104594D-07
-9.438304330D-12 2.725038297D-16                  3.392428060D+04-6.679585350D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6725.403
 1.779004264D+08-1.082328257D+05 2.810778365D+01-2.975232262D-03 1.854997534D-07
-5.796231540D-12 7.191720164D-17                  8.890942630D+05-2.181728151D+02
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O+                Martin,1993. Gordon,1999.
 3 g 8/97 O   1.00E  -1.00     0.00     0.00     0.00 0   15.9988514     1568787.228
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.879352842D+05 4.393376760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-2.166513208D+05 6.665456150D+02 1.702064364D+00 4.714992810D-04-1.427131823D-07
 2.016595903D-11-9.107157762D-16                 1.837191966D+05 1.005690382D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-2.143835383D+08 1.469518523D+05-3.680864540D+01 5.036164540D-03-3.087873854D-07
 9.186834870D-12-1.074163268D-16                -9.614208960D+05 3.426193080D+02
O-                Gurvich,1989 pt1 p93. Hotop,1985. Gordon,1999.
 3 g 1/97 O   1.00E   1.00     0.00     0.00     0.00 0   15.9999486      101846.192
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6570.792
-5.695857110D+03 1.099287334D+02 2.184719661D+00 5.326359800D-04-5.298878440D-07
 2.870216236D-10-6.524692740D-14                 1.093287498D+04 6.729863860D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6570.792
 9.769363180D+03 7.159604780D+00 2.494961726D+00 1.968240938D-06-4.304174850D-10
 4.912083080D-14-2.271600083D-18                 1.149554438D+04 4.837036440D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6570.792
 5.662391000D+02 7.572340320D+00 2.498352500D+00 1.862632395D-07-1.151227211D-11
 3.688814210D-16-4.793297600D-21                 1.148426000D+04 4.813406590D+00
OD                D0(OH)with ZPEadj. Gurvich,1989 pt1 p135 pt2 p47.
 2 g 4/02 O   1.00D   1.00     0.00     0.00     0.00 0   18.0135020      35172.008
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8999.108
 2.118691536D+04-2.785982360D+02 5.456210120D+00-6.148119830D-03 9.117670560D-06
-5.527812710D-09 1.239794711D-12                 4.464878250D+03-7.616618910D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8999.108
 7.832473160D+05-2.532992554D+03 5.952124650D+00-3.743595280D-04 4.959527620D-08
 3.454454730D-12-7.380626800D-16                 1.930492973D+04-1.568898441D+01
OD-               Gurvich,1989 pt1 p137 pt2 p48.
 2 g 4/02 O   1.00D   1.00E   1.00     0.00     0.00 0   18.0140506    -147557.896
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8642.104
 5.606128320D+04-7.514156150D+02 7.544188470D+00-1.092083064D-02 1.503688938D-05
-9.351665840D-09 2.246466046D-12 0.000000000D+00-1.515707370D+04-2.106498377D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8642.104
 3.029467029D+05-1.079684654D+03 4.211417380D+00 6.260830070D-04-2.411665054D-07
 4.248425540D-11-2.387099102D-15 0.000000000D+00-1.188935343D+04-4.724898790D+00
OH                D0(H-OH): Ruscic,2002. Gurvich,1978 pt1 p110 pt2 p37.
 3 g 4/02 O   1.00H   1.00     0.00     0.00     0.00 0   17.0073400      37278.206
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8813.106
-1.998858990D+03 9.300136160D+01 3.050854229D+00 1.529529288D-03-3.157890998D-06
 3.315446180D-09-1.138762683D-12                 2.991214235D+03 4.674110790D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8813.106
 1.017393379D+06-2.509957276D+03 5.116547860D+00 1.305299930D-04-8.284322260D-08
 2.006475941D-11-1.556993656D-15                 2.019640206D+04-1.101282337D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8813.106
 2.847234193D+08-1.859532612D+05 5.008240900D+01-5.142374980D-03 2.875536589D-07
-8.228817960D-12 9.567229020D-17                 1.468393908D+06-4.023555580D+02
OH+               IP: Wiedmann,1992. Gurvich,1978 v1 pt2 p39.
 3 g 4/02 O   1.00H   1.00E  -1.00     0.00     0.00 0   17.0067914    1299213.203
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8603.103
 6.031630860D+04-7.573520300D+02 7.307752930D+00-9.506881670D-03 1.202555795D-05
-6.829026100D-09 1.501588659D-12                 1.589262158D+05-1.950106996D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8603.103
 5.040729100D+05-1.380052958D+03 4.125462200D+00 8.331948840D-04-3.442856290D-07
 6.792853950D-11-4.363872130D-15                 1.643839235D+05-3.997058490D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8603.103
 1.158286700D+09-6.841280390D+05 1.576194558D+02-1.618421339D-02 8.846128780D-07
-2.475038507D-11 2.807730875D-16                 5.616597180D+06-1.351879042D+03
OH-               Gurvich,1989 pt1 p118 pt2 p32.
 2 g 4/02 O   1.00H   1.00E   1.00     0.00     0.00 0   17.0078886    -145256.196
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8606.104
 2.910880827D+04-3.216904940D+02 4.851029050D+00-2.579035357D-03 2.004980024D-06
-7.956852960D-11-2.320495634D-13                -1.688886234D+04-7.121591300D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8606.104
 4.711331170D+05-8.572336690D+02 3.166181210D+00 1.233581296D-03-3.999244580D-07
 6.239081670D-11-3.354343220D-15                -1.224849139D+04 1.487736260D+00
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O2                Ref-Elm. Gurvich,1989 pt1 p94 pt2 p9.
 3 tpis89 O   2.00    0.00    0.00    0.00    0.00 0   31.9988000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.104
-3.425563420D+04 4.847000970D+02 1.119010961D+00 4.293889240D-03-6.836300520D-07
-2.023372700D-09 1.039040018D-12                -3.391454870D+03 1.849699470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.104
-1.037939022D+06 2.344830282D+03 1.819732036D+00 1.267847582D-03-2.188067988D-07
 2.053719572D-11-8.193467050D-16                -1.689010929D+04 1.738716506D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.104
 4.975294300D+08-2.866106874D+05 6.690352250D+01-6.169959020D-03 3.016396027D-07
-7.421416600D-12 7.278175770D-17                 2.293554027D+06-5.530621610D+02
O2+               Gurvich,1989 pt1 p98 pt2 p11.
 3 tpis89 O   2.00E  -1.00    0.00    0.00    0.00 0   31.9982514    1171828.436
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9311.112
-8.607205450D+04 1.051875934D+03-5.432380470D-01 6.571166540D-03-3.274263750D-06
 5.940645340D-11 3.238784790D-13                 1.345544668D+05 2.902709750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9311.112
 7.384654880D+04-8.459559540D+02 4.985164160D+00-1.611010890D-04 6.427083990D-08
-1.504939874D-11 1.578465409D-15                 1.446321044D+05-5.811230650D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9311.112
-1.562125524D+09 1.161406778D+06-3.302504720D+02 4.710937520D-02-3.354461380D-06
 1.167968599D-10-1.589754791D-15                -8.857866270D+06 2.852035602D+03
O2-               Gurvich,1989 pt1 p100 pt2 p13.
 2 g11/99 O   2.00E   1.00    0.00    0.00    0.00 0   31.9993486     -48027.921
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9349.611
 1.883874344D+04 1.149551768D+02 1.518876821D+00 8.016111380D-03-9.850571030D-06
 6.044196210D-09-1.486439845D-12                -7.101538760D+03 1.501210380D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9349.611
-5.655208050D+04-2.367815862D+02 4.675833670D+00-2.197245300D-05 1.711509280D-08
-1.757645062D-12 8.248172790D-17                -5.960177750D+03-2.436885556D+00
O3                Gurvich,1989 pt1 p101 pt2 p15.
 2 g 8/01 O   3.00    0.00    0.00    0.00    0.00 0   47.9982000     141800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10366.305
-1.282314507D+04 5.898216640D+02-2.547496763D+00 2.690121526D-02-3.528258340D-05
 2.312290922D-08-6.044893270D-12                 1.348368701D+04 3.852218580D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10366.305
-3.869662480D+07 1.023344994D+05-8.961551600D+01 3.706144970D-02-4.137638740D-06
-2.725018591D-10 5.248188110D-14                -6.517918180D+05 7.029109520D+02
P                 Hf:Cox,1989. Martin,1985. Gordon,1999.
 3 g 5/97 P   1.00    0.00    0.00    0.00    0.00 0   30.9737610     316500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 5.040866570D+01-7.639418650D-01 2.504563992D+00-1.381689958D-05 2.245585515D-08
-1.866399889D-11 6.227063395D-15                 3.732421910D+04 5.359303481D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.261794642D+06-4.559838190D+03 8.918079310D+00-4.381401460D-03 1.454286224D-06
-2.030782763D-10 1.021022887D-14                 6.541723960D+04-3.915974795D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.215392545D+07-4.566911180D+04 2.837245428D+01-4.483244040D-03 3.579413080D-07
-1.255311557D-11 1.590290483D-16                 3.370905760D+05-2.056960928D+02
P+                Martin,1985. Gordon,1999.
 3 g 4/97 P   1.00E  -1.00    0.00    0.00    0.00 0   30.9732124    1336453.460
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8141.860
-7.316908110D+04 9.627979140D+02-3.693938050D-01 4.766778340D-03-4.574768580D-06
 2.371262331D-09-5.131314900D-13                 1.549406849D+05 2.376640762D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8141.860
-5.594249360D+05 1.722576545D+03 8.430381090D-01 6.287368940D-04-6.317195460D-08
-1.810842484D-12 4.318112570D-16                 1.490493431D+05 1.845275207D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8141.860
 1.362531054D+07-8.717502380D+03 4.747426280D+00-1.620871933D-04-3.935548100D-10
 4.845613020D-13-7.448402970D-18                 2.284649718D+05-1.346454894D+01
P-                Hotop,1985. Gordon,1999.
 3 g 4/97 P   1.00E   1.00    0.00    0.00    0.00 0   30.9743096     238826.765
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6747.865
-1.008949093D+04 1.826468403D+02 1.962456304D+00 9.197377540D-04-9.214998630D-07
 5.012872360D-10-1.142677121D-13                 2.703082432D+04 9.478137822D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6747.865
 1.543488016D+04 9.495009340D+00 2.493170861D+00 2.700167711D-06-5.949210390D-10
 6.823766290D-14-3.166959910D-18                 2.797572693D+04 6.246793872D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6747.865
 1.724147889D+03 1.074832503D+01 2.497654940D+00 2.655333078D-07-1.642839012D-11
 5.268015350D-16-6.849362660D-21                 2.795482976D+04 6.215849262D+00
```

Appendix D (*continued*)

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PCL                Gurvich,1989 pt1 p431 pt2 p282.
 2 tpis89 P   1.00CL  1.00     0.00     0.00     0.00 0   66.4267610      134615.112
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9291.112
 3.488861700D+04-5.603119340D+02 6.264568480D+00-3.183364370D-03 3.495326840D-06
-2.091034291D-09 5.418758600D-13                 1.774653764D+04-8.074572148D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9291.112
-3.471681510D+05 9.935557930D+02 3.399430270D+00 4.019711700D-04 8.295588390D-08
-3.090212484D-11 2.106384858D-15                 8.433591150D+03 1.064902238D+01
PCL2               Gurvich,1989 pt1 p432 pt2 p283.
 2 tpis89 P   1.00CL  2.00     0.00     0.00     0.00 0  101.8797610      -54292.353
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12248.757
 5.190084500D+04-1.060904200D+03 1.058549940D+01-6.879917530D-03 7.620773180D-06
-4.530115470D-09 1.116671660D-12                -3.220331180D+03-2.753518359D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12248.757
-8.349833970D+04-2.625249470D+01 7.020361810D+00-8.388768680D-06 1.896784740D-09
-2.214879920D-13 1.041653550D-17                -8.742993680D+03-6.234023190D+00
PCL2-              Gurvich,1989 pt1 p433 pt2 p284.
 2 tpis89 P   1.00CL  2.00E   1.00     0.00     0.00 0  101.8803096     -356285.253
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12453.247
 4.934832770D+04-9.601590540D+02 9.884769700D+00-4.950202950D-03 4.946217870D-06
-2.678675201D-09 6.076723610D-13                -3.998072400D+04-2.413131695D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12453.247
-8.564986760D+04-3.185555940D+01 7.024494960D+00-1.002251172D-05 2.253747944D-09
-2.619657192D-13 1.227059658D-17                -4.503811430D+04-6.721522361D+00
PCL3               Gurvich,1989 pt1 p433 pt2 p285.
 2 tpis89 P   1.00CL  3.00     0.00     0.00     0.00 0  137.3327610     -289500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15932.466
 7.717745470D+04-1.617650860D+03 1.536080470D+01-1.011077050D-02 1.103408340D-05
-6.476121020D-09 1.579151140D-12                -2.955893640D+04-5.244338688D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15932.466
-1.333076930D+05-4.145883210D+01 1.003186060D+01-1.301946160D-05 2.922916890D-09
-3.391869240D-13 1.586425530D-17                -3.800336680D+04-2.050737678D+01
PCL5               Gurvich,1989 pt1 p435 pt2 p286.
 2 tpis89 P   1.00CL  5.00     0.00     0.00     0.00 0  208.2387610     -376000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23305.466
 1.029070200D+05-2.515707460D+03 2.430114970D+01-1.564610690D-02 1.709873030D-05
-1.006011430D-08 2.460158790D-12                -3.722582370D+04-9.816335170D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23305.466
-2.255906890D+05-6.938542820D+01 1.605359630D+01-2.202156960D-05 4.971392290D-09
-5.799860050D-13 2.725970770D-17                -5.034234220D+04-4.872454870D+01
PF                 Gurvich,1989 pt1 p425 pt2 p276.
 2 tpis89 P   1.00F   1.00     0.00     0.00     0.00 0   49.9721642      -47944.793
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8891.107
 2.227866728D+04-1.727508706D+02 3.085366934D+00 5.489718230D-03-8.247972540D-06
 5.868882910D-09-1.617252113D-12                -5.809279650D+03 7.709718850D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8891.107
-1.132572282D+06 3.200038550D+03 7.780502370D-01 1.969518902D-03-4.365818970D-07
 5.243648570D-11-2.618755712D-15                -2.766773009D+04 2.759312302D+01
PF+                Chase,1998 p1086.
 3 j 6/77 P   1.00F   1.00E  -1.00     0.00     0.00 0   49.9716156      901518.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9429.848
-1.779138157D+04 3.909991270D+02 1.257434156D+00 7.861363750D-03-9.342312680D-06
 5.630915650D-09-1.370669924D-12                 1.054873882D+05 1.901676576D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9429.848
-4.011525180D+04-1.597504413D+02 4.621397480D+00-2.378072183D-05 1.431831329D-08
-2.300109157D-12 1.694069882D-16                 1.078633756D+05-4.072343950D-02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9429.848
-2.628686921D+07 1.300876535D+04 2.564713658D+00 3.269650350D-05 1.867188317D-08
-9.293307220D-13 1.456723674D-17                -2.640503508D+02 1.921588661D+01
PF-                Chase,1998 p1087.
 3 j 6/77 P   1.00F   1.00E   1.00     0.00     0.00 0   49.9727128     -164046.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9515.643
 7.705210950D+03-1.152432706D+02 4.254952310D+00 1.163521526D-03-1.627947259D-06
 1.084382815D-09-2.809490132D-13                -2.035558966D+04 2.217923793D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9515.643
-1.303793388D+05 2.715526386D+02 4.137619810D+00 2.728610614D-04-7.644416250D-08
 1.182073001D-11-6.083906640D-16                -2.290799827D+04 3.748526100D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9515.643
-2.589702487D+07 2.274827883D+04-2.913204829D+00 1.134351740D-03-7.184766090D-08
 2.254067861D-12-2.781608692D-17                -1.940751937D+05 6.372454240D+01
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PFCL              Gurvich,1989 pt1 p437 pt2 p288.
 2 tpis89 P   1.00F   1.00CL  1.00    0.00    0.00 0   85.4251642    -283184.119
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11630.381
 5.490188530D+04-8.658679480D+02 7.944467650D+00 9.503779100D-04-3.339090210D-06
 3.023977817D-09-9.450377540D-13                -3.132843217D+04-1.440426886D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11630.381
-1.282143211D+05-9.739043550D+01 7.072661660D+00-2.903614134D-05 6.408504490D-09
-7.338993770D-13 3.396723170D-17                -3.600649260D+04-7.626493035D+00
PFCL-             Gurvich,1989 pt1 p438 pt2 p289.
 2 tpis89 P   1.00F   1.00CL  1.00E   1.00    0.00 0   85.4257128    -529269.107
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11742.793
 8.934336850D+04-1.266972513D+03 9.912194530D+00-3.877928300D-03 3.036692411D-06
-1.296559380D-09 2.324226580D-13                -5.894505710D+04-2.617050460D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11742.793
-1.231565150D+05-9.765861110D+01 7.074029570D+00-2.997070692D-05 6.685280620D-09
-7.722262200D-13 3.599382300D-17                -6.558817220D+04-8.208878059D+00
PFCL2             Gurvich,1989 pt1 p440 pt2 p292.
 2 tpis89 P   1.00F   1.00CL  2.00    0.00    0.00 0  120.8781642    -511925.340
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14867.760
 8.266560560D+04-1.512138928D+03 1.303404207D+01-2.903247162D-03 7.836652970D-07
 6.458340660D-10-3.737641820D-13                -5.644237870D+04-4.100905668D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14867.760
-1.864589813D+05-1.148004379D+02 1.008599754D+01-3.447456520D-05 7.627972010D-09
-8.753097430D-13 4.057788350D-17                -6.450472190D+04-2.174054563D+01
PFCL4             Gurvich,1989 pt1 p442 pt2 p295.
 2 tpis89 P   1.00F   1.00CL  4.00    0.00    0.00 0  191.7841642    -635016.440
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21733.860
 1.412071573D+05-2.882471080D+03 2.387345233D+01-1.239510207D-02 1.141290085D-05
-5.705483820D-09 1.195229703D-12                -6.613478650D+04-9.859693550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21733.860
-2.954375880D+05-1.325154294D+02 1.610005380D+01-4.035359170D-05 8.971130740D-09
-1.033288810D-12 4.804468350D-17                -8.135719400D+04-5.062403920D+01
PF2               Gurvich,1989 pt1 p426 pt2 p277.
 2 tpis89 P   1.00F   2.00    0.00    0.00    0.00 0   68.9705674    -513103.659
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11081.447
 5.524765720D+04-6.280517800D+02 5.137437920D+00 9.120673350D-03-1.468773760D-05
 1.081268450D-08-3.064944490D-12                -5.977541470D+04-1.689589472D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11081.447
-1.708467120D+05-1.692051540D+02 7.125491600D+00-4.990852850D-05 1.097335230D-08
-1.252870260D-12 5.784791140D-17                -6.338295840D+04-1.041715673D+01
PF2-              Gurvich,1989 pt1 p426 pt2 p278.
 2 tpis89 P   1.00F   2.00E   1.00    0.00    0.00 0   68.9711160    -709337.947
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11044.553
 1.404793057D+05-1.699945753D+03 1.036823971D+01-3.599587690D-03 1.961925800D-06
-3.829329870D-10-3.375549520D-14                -7.810434510D+04-3.217375182D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11044.553
-1.653976056D+05-1.640604822D+02 7.124091520D+00-5.015431400D-05 1.117302152D-08
-1.289308601D-12 6.004706670D-17                -8.700223320D+04-1.109074866D+01
PF2CL             Gurvich,1989 pt1 p439 pt2 p290.
 2 tpis89 P   1.00F   2.00CL  1.00    0.00    0.00 0  104.4235674    -735076.682
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13876.318
 8.397590160D+04-1.318075883D+03 1.017203515D+01 5.571231220D-03-1.100920478D-05
 8.726383180D-09-2.567714099D-12                -8.381656170D+04-2.766012951D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13876.318
-2.409281185D+05-2.033484670D+02 1.015150769D+01-6.048367310D-05 1.333942001D-08
-1.526772528D-12 7.063339180D-17                -9.101110590D+04-2.417825549D+01
PF2CL3            Gurvich,1989 pt1 p442 pt2 p294.
 2 tpis89 P   1.00F   2.00CL  3.00    0.00    0.00 0  175.3295674    -878744.962
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20165.238
 1.842099543D+05-3.334402390D+03 2.388510873D+01-1.030943175D-02 7.356504220D-06
-2.498621785D-09 2.513997646D-13                -9.279549890D+04-1.027991502D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20165.238
-3.655272540D+05-2.029694160D+02 1.615238015D+01-6.118796570D-05 1.355610375D-08
-1.557129640D-12 7.224359970D-17                -1.104941533D+05-5.387308191D+01
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PF3                Gurvich,1989 pt1 p427 pt2 p279.
 2 tpis89 P   1.00F   3.00    0.00    0.00    0.00 0   87.9689706    -957400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12936.493
 8.480984480D+04-1.102340691D+03 7.160715110D+00 1.438278338D-02-2.318137222D-05
 1.702244315D-08-4.810991950D-12                -1.111837495D+05-1.457652362D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12936.493
-2.957040675D+05-2.997689931D+02 1.022297023D+01-8.890263450D-05 1.958901359D-08
-2.240491075D-12 1.035952523D-16                -1.173743464D+05-2.777419177D+01
PF3CL2             Gurvich,1989 pt1 p441 pt2 p293.
 2 tpis89 P   1.00F   3.00CL  2.00    0.00    0.00 0   158.8749706   -1122022.916
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19047.184
 1.822497206D+05-3.089610245D+03 2.067710388D+01-1.168732391D-03-5.020540740D-06
 5.804573350D-09-1.965367906D-12                -1.228120667D+05-8.627977355D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19047.184
-4.223838050D+05-3.207965220D+02 1.624013000D+01-9.623655310D-05 2.129279712D-08
-2.443515401D-12 1.132904350D-16                -1.392642151D+05-5.531285745D+01
PF4CL              Gurvich,1989 pt1 p439 pt2 p291.
 2 tpis89 P   1.00F   4.00CL  1.00    0.00    0.00 0   142.4203738   -1364909.395
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18320.605
 1.804240323D+05-2.741096618D+03 1.680192838D+01 9.919315250D-03-2.025636171D-05
 1.617979147D-08-4.772611520D-12                -1.532382587D+05-6.679119965D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18320.605
-4.781140040D+05-4.264812830D+02 1.631812121D+01-1.271374903D-04 2.806715254D-08
-3.215166300D-12 1.488512118D-16                -1.680488362D+05-5.735844805D+01
PF5                Gurvich,1989 pt1 p429 pt2 p280.
 2 tpis89 P   1.00F   5.00    0.00    0.00    0.00 0   125.9657770   -1593300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16537.609
 1.855778473D+05-2.436979828D+03 1.201012406D+01 2.339343049D-02-3.813944410D-05
 2.796136412D-08-7.870704880D-12                -1.814566568D+05-4.486488740D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16537.609
-5.668727840D+05-6.677917910D+02 1.649789569D+01-1.990099440D-04 4.395007100D-08
-5.036849540D-12 2.332945909D-16                -1.944321623D+05-6.261721040D+01
PH                 Gurvich,1989 pt1 p420 pt2 p272.
 2 tpis89 P   1.00H   1.00    0.00    0.00    0.00 0   31.9817010     230752.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8648.104
 2.273633198D+04-3.972674060D+02 6.233697660D+00-9.181784600D-03 1.523328123D-05
-1.085888585D-08 2.929760547D-12                2.852768404D+04-1.095191197D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8648.104
 7.814730650D+05-3.038451204D+03 7.467481020D+00-1.837522255D-03 7.165947700D-07
-1.142128853D-10 6.175410560D-15                4.536260180D+04-2.467298140D+01
PH2                Gurvich,1989 pt1 p422 pt2 p273.
 2 tpis89 P   1.00H   2.00    0.00    0.00    0.00 0   32.9896410     119553.470
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9981.571
 1.555268372D+04-1.841602025D+02 4.895896040D+00-3.495436600D-03 1.053418945D-05
-8.377562920D-09 2.270766150D-12                1.409839468D+04-2.210564792D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9981.571
 1.127884913D+06-4.715238250D+03 1.021498300D+01-1.167573820D-03 2.150542671D-07
-1.624213739D-11 3.766225240D-16                4.183074630D+04-4.231623250D+01
PH2-               Gurvich,1989 pt1 p423 pt2 p274.
 2 tpis89 P   1.00H   2.00E   1.00    0.00    0.00 0   32.9901896     -9265.418
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9960.082
 6.950684490D+04-7.719162910D+02 7.383537620D+00-8.522947210D-03 1.474476507D-05
-9.847160810D-09 2.413107871D-12                1.582295850D+03-1.761306419D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9960.082
 1.382525815D+06-5.213400670D+03 1.021694832D+01-1.116316349D-03 2.215004171D-07
-2.338005187D-11 1.015580932D-15                2.990683733D+04-4.378711585D+01
PH3                Chase,1998 p1348.
 2 j 6/62 P   1.00H   3.00    0.00    0.00    0.00 0   33.9975810     5439.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10136.622
-6.384325340D+03 4.057567410D+02-1.565680086D-01 1.338380613D-02-8.275391430D-06
 3.024360831D-09-6.421764630D-13               -2.159842124D+03 2.385561888D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10136.622
 1.334801106D+06-6.725463520D+03 1.445857073D+01-1.639736883D-03 3.409218570D-07
-3.736272080D-11 1.672947506D-15                3.910325710D+04-7.198781190D+01
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Appendix D (*continued*)

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PN                Gurvich,1989 pt1 p446 pt2 p299.
 2 tpis89 P   1.00N   1.00     0.00     0.00     0.00 0   44.9804610     171487.305
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8702.105
-5.103203840D+04 8.202926680D+02-1.392772765D+00 1.287989789D-02-1.401425371D-05
 7.775633460D-09-1.751539330D-12                  1.573226520D+04 3.251070633D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8702.105
-2.495625593D+05 1.760438830D+02 4.144121960D+00 2.478018097D-04-5.674896300D-08
 4.263645120D-12 3.063920924D-16                  1.770317267D+04 1.325517397D+00
PO                Gurvich,1989 pt1 p404 pt2 p258.
 2 tpis89 P   1.00O   1.00     0.00     0.00     0.00 0   46.9731610     -27857.687
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9390.113
-6.845754060D+04 1.141295708D+03-2.779556060D+00 1.678458047D-02-1.974879516D-05
 1.192602320D-08-2.927460912D-12                 -9.847745040D+03 4.184328297D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9390.113
-3.366667440D+05 6.229355840D+02 3.565605460D+00 6.516620720D-04-2.061770841D-07
 3.184413230D-11-1.573691908D-15                 -8.939790390D+03 6.954859188D+00
PO-               Gurvich,1989 pt1 p407 pt2 p259.
 2 tpis89 P   1.00O   1.00E    1.00     0.00     0.00 0   46.9737096     -140067.094
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8778.106
 5.434346320D+04-4.123623550D+02 3.746483880D+00 3.858636470D-03-5.963343040D-06
 4.278286360D-09-1.139722989D-12                 -1.555810937D+04 3.404436468D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8778.106
-8.480294780D+02 3.470544870D+02 2.877890167D+00 1.622182445D-03-4.870190990D-07
 6.645752270D-11-3.395703760D-15                 -1.987209540D+04 1.075444355D+01
POCL3             Gurvich,1989 pt1 p436 pt2 p287.
 2 tpis89 P   1.00O   1.00CL   3.00     0.00     0.00 0  153.3321610     -568400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17715.956
 4.793788160D+04-1.270388280D+03 1.367716460D+01 1.082672100D-03-1.736104060D-06
 8.460890640D-10-1.174661330D-13                 -6.507571880D+04-4.314705941D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17715.956
-2.185937970D+05-5.080269680D+02 1.337784650D+01-1.510731050D-04 3.340986780D-08
-3.835329760D-12 1.779329880D-16                 -7.009315090D+04-3.984746301D+01
POFCL2            Gurvich,1989 pt1 p444 pt2 p297.
 2 tpis89 P   1.00O   1.00F   1.00CL  2.00     0.00 0  136.8775642     -793889.312
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16454.188
 4.694061560D+04-1.069242600D+03 1.071284279D+01 9.491183300D-03-1.306412424D-05
 8.426906020D-09-2.140294969D-12                 -9.274894990D+04-2.815077719D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16454.188
-2.707647503D+05-6.556502270D+02 1.348668421D+01-1.942765035D-04 4.291184490D-08
-4.921844800D-12 2.282079808D-16                 -9.654392140D+04-4.164963494D+01
POF2CL            Gurvich,1989 pt1 p443 pt2 p296.
 2 tpis89 P   1.00O   1.00F   2.00CL  1.00     0.00 0  120.4229674    -1022607.040
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14896.360
 5.226438160D+04-9.691037700D+02 7.963635980D+00 1.755599796D-02-2.398693997D-05
 1.572376747D-08-4.079746000D-12                 -1.202656893D+05-1.593967075D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14896.360
-3.347086590D+05-8.176104810D+02 1.360664320D+01-2.420426112D-04 5.343712720D-08
-6.126461350D-12 2.839570116D-16                 -1.233401194D+05-4.496103437D+01
POF3              Gurvich,1989 pt1 p430 pt2 p281.
 2 tpis89 P   1.00O   1.00F   3.00     0.00     0.00 0  103.9683706    -1252000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14166.349
 2.966030710D+04-4.276705750D+02 3.669146100D+00 2.839493780D-02-3.768318000D-05
 2.449104540D-08-6.341972870D-12                 -1.501124530D+05 5.160417996D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14166.349
-3.690602420D+05-1.005552540D+03 1.374529940D+01-2.971037110D-04 6.554526640D-08
-7.509987330D-12 3.478969910D-16                 -1.499761730D+05-4.882214181D+01
PO2               Gurvich,1989 pt1 p408 pt2 p260.
 2 tpis89 P   1.00O   2.00     0.00     0.00     0.00 0   62.9725610     -281527.237
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10512.866
-6.372698220D+04 1.036741044D+03-2.877797967D+00 2.278134083D-02-2.567920328D-05
 1.465060412D-08-3.387996700D-12                 -3.993544720D+04 4.425309380D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10512.866
 4.926210990D+05-2.605465745D+03 9.517605610D+00-1.180371565D-03 2.532912819D-07
-1.789964539D-11 1.800381054D-16                 -2.028884763D+04-2.969743125D+01
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PO2-              Gurvich,1989 pt1 p409 pt2 p261.
 2 tpis89 P   1.00O   2.00E   1.00    0.00    0.00 0   62.9731096    -597623.751
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 2.702423135D+04 2.939956284D+01 1.162686114D+00 1.599897972D-02-1.979229263D-05
 1.208847527D-08-2.956640480D-12                -7.285946270D+04 1.963118182D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 1.628679152D+06-5.989199980D+03 1.369318836D+01-3.623843790D-03 9.488198340D-07
-1.040308759D-10 4.019033660D-15                -3.685959500D+04-5.956796220D+01
PS                Gurvich,1989 pt1 p444 pt2 p298.
 2 tpis89 P   1.00S   1.00    0.00    0.00    0.00 0   63.0387610     150431.316
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9616.116
-7.689786800D+02-4.637824070D+01 4.104649170D+00 1.555262273D-03-2.315757288D-06
 1.661425178D-09-4.631238400D-13                1.707875808D+04 4.230652171D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9616.116
-2.702729081D+05 8.883548220D+02 3.169190120D+00 1.022480817D-03-3.803740480D-07
 7.019861880D-11-4.269122310D-15                1.121510462D+04 1.147334049D+01
P2                Gurvich,1989 pt1 p398 pt2 p255.
 2 tpis89 P   2.00    0.00    0.00    0.00    0.00 0   61.9475220     144000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8904.107
 3.053922510D+04-3.246177590D+02 4.022463810D+00 3.232094790D-03-5.511052450D-06
 4.195572930D-09-1.215032180D-12                1.796910870D+04 1.645350331D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8904.107
-7.806936490D+05 2.307910870D+03 1.411743130D+00 2.108237420D-03-7.360856620D-07
 1.259360120D-10-7.079752490D-15                1.329824740D+03 2.169741365D+01
P2O3              Gurvich,1989 pt1 p410 pt2 p262.
 2 tpis89 P   2.00O   3.00    0.00    0.00    0.00 0  109.9457220    -684645.274
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16094.881
-6.645753890D+04 7.580900550D+02 9.888436770D-01 2.859878730D-02-3.231142110D-05
 1.834525170D-08-4.212489300D-12                -8.820036740D+04 2.689914458D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16094.881
-2.175344110D+05-1.369902000D+03 1.401142960D+01-4.023856960D-04 8.868345780D-08
-1.015657280D-11 4.704356060D-16                -7.922757000D+04-4.739487232D+01
P2O4              Gurvich,1989 pt1 p411 pt2 p263.
 2 tpis89 P   2.00O   4.00    0.00    0.00    0.00 0  125.9451220    -933754.627
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17325.580
-4.376091260D+04 4.905102830D+02 9.643649370D-01 3.886073580D-02-4.675509220D-05
 2.812625630D-08-6.824406100D-12                -1.168997790D+05 2.379582767D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17325.580
-3.670114860D+05-1.638423730D+03 1.721188610D+01-4.826580150D-04 1.064461900D-07
-1.219610070D-11 5.650654580D-16                -1.090435930D+05-6.714276593D+01
P2O5              Gurvich,1989 pt1 p411 pt2 p264.
 2 tpis89 P   2.00O   5.00    0.00    0.00    0.00 0  141.9445220   -1124370.354
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22049.905
-2.999159220D+04-4.594506590D+01 6.987486830D+00 2.883302970D-02-3.104509530D-05
 1.643868680D-08-3.467942300D-12                -1.381901400D+05-3.400572711D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22049.905
-3.247080160D+05-2.016975080D+03 2.048699340D+01-5.910641150D-04 1.301993020D-07
-1.490682940D-11 6.903573410D-16                -1.306290160D+05-8.031642952D+01
P3                Gurvich,1989 pt1 p402 pt2 p256.
 2 tpis89 P   3.00    0.00    0.00    0.00    0.00 0   92.9212830     210000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12005.602
 4.693358950D+04-8.643589320D+02 8.734247530D+00 1.094534560D-05-1.998573320D-06
 2.096750510D-09-6.922889710D-13                 2.774847340D+04-2.063587261D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12005.602
-1.253513060D+05-8.306734620D+01 7.561956770D+00-2.474403950D-05 5.457276930D-09
-6.244660570D-13 2.887724220D-17                 2.308722280D+04-1.228310621D+01
P3O6              Gurvich,1989 pt1 p412 pt2 p265.
 2 tpis89 P   3.00O   6.00    0.00    0.00    0.00 0  188.9176830   -1575681.029
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23439.282
 2.014493813D+05-3.053488073D+03 1.602114098D+01 4.316889900D-02-6.376544260D-05
 4.422867920D-08-1.200020334D-11                -1.776503811D+05-6.556267890D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23439.282
-8.787968100D+05-1.651988071D+03 2.772258397D+01-4.859326700D-04 1.067867708D-07
-1.218015776D-11 5.614911960D-16                -1.909165548D+05-1.220665277D+02
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P4                Gurvich,1989 pt1 p402 pt2 p257.
 2 tpis89 P   4.00     0.00     0.00     0.00     0.00 0  123.8950440       58900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            14108.648
 1.205141850D+05-2.345711790D+03 1.773946550D+01-1.456314970D-02 1.587594090D-05
-9.314710310D-09 2.271491670D-12                 1.608846480D+04-7.088590647D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            14108.648
-1.858705860D+05-6.284546890D+01 1.004844880D+01-1.987668850D-05 4.482408440D-09
-5.226103670D-13 2.455791290D-17                 3.848210920D+03-2.477297797D+01
P406              Gurvich,1989 pt1 p413 pt2 p266.
 2 tpis89 P   4.00O   6.00     0.00     0.00     0.00 0  219.8914440    -1606000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            24797.523
 3.760894750D+05-5.685832620D+03 2.914225450D+01 2.251532120D-02-4.510269630D-05
 3.588312690D-08-1.057572060D-11                -1.688562480D+05-1.451359851D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            24797.523
-1.008997240D+06-8.872753990D+02 2.866064830D+01-2.636018940D-04 5.810940720D-08
-6.648086960D-12 3.074391930D-16                -1.997138900D+05-1.281853821D+02
P407              Gurvich,1989 pt1 p414 pt2 p267.
 2 tpis89 P   4.00O   7.00     0.00     0.00     0.00 0  235.8908440    -1984448.045
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            26372.317
 3.218586960D+05-4.871444730D+03 2.454417068D+01 4.015509550D-02-6.524197150D-05
 4.756554180D-08-1.332975491D-11                -2.184517427D+05-1.181504792D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            26372.317
-1.102947375D+06-1.511077128D+03 3.210979500D+01-4.371803760D-04 9.516639610D-08
-1.075204176D-11 4.911025680D-16                -2.429096540D+05-1.473140859D+02
P408              Gurvich,1989 pt1 p415 pt2 p268.
 2 tpis89 P   4.00O   8.00     0.00     0.00     0.00 0  251.8902440    -2302214.078
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            27946.336
 2.719326942D+05-4.118600390D+03 2.028714235D+01 5.685416990D-02-8.400739630D-05
 5.823389060D-08-1.578647160D-11                -2.604539703D+05-9.407162070D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            27946.336
-1.173177311D+06-2.200632995D+03 3.563010130D+01-6.489849740D-04 1.429623989D-07
-1.635821725D-11 7.571070760D-16                -2.783843144D+05-1.679636960D+02
P409              Gurvich,1989 pt1 p416 pt2 p269.
 2 tpis89 P   4.00O   9.00     0.00     0.00     0.00 0  267.8896440    -2613979.111
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            29521.355
 2.199916395D+05-3.336464940D+03 1.586413106D+01 7.402452330D-02-1.034835052D-04
 6.944438320D-08-1.840733450D-11                -3.018742692D+05-6.997967670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            29521.355
-1.233696783D+06-2.917032808D+03 3.917757110D+01-8.736402980D-04 1.937914895D-07
-2.230510118D-11 1.037248818D-15                -3.129637516D+05-1.897176420D+02
P4O10             Gurvich,1989 pt1 p419 pt2 p271.
 2 tpis89 P   4.00O  10.00     0.00     0.00     0.00 0  283.8890440    -2906223.447
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            31096.553
 1.670142268D+05-2.540243300D+03 1.136853403D+01 9.137812160D-02-1.231990626D-04
 8.081032230D-08-2.106787011D-11                -3.410151910D+05-4.643431340D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            31096.553
-1.337201132D+06-3.516382330D+03 4.260403310D+01-1.037406404D-03 2.287613089D-07
-2.620219946D-11 1.213529528D-15                -3.459515050D+05-2.115498906D+02
Pb                Hf:Gurvich,1991. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 8/97 PB  1.00     0.00     0.00     0.00     0.00 0  207.2000000     195200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             6197.428
 1.213382285D+03-1.906116019D+01 2.619299546D+00-3.829519610D-04 6.688180450D-07
-6.061231080D-10 2.240022429D-13                 2.282096238D+04 6.201369200D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             6197.428
-9.084313070D+06 2.672673180D+04-2.626244039D+01 1.358282305D-02-2.685523566D-06
 2.352432800D-10-7.324114532D-15                -1.481650666D+05 2.154011624D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             6197.428
 5.325474970D+08-2.751419152D+05 6.303031930D+01-6.813672740D-03 4.447489610D-07
-1.519361678D-11 2.043475665D-16                 2.243651683D+06-5.225649900D+02
Pb+               Moore1971. Moore,1970a. Gordon,1999.
 3 g10/97 PB  1.00E  -1.00     0.00     0.00     0.00 0  207.1994514     916996.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             6197.428
 9.486689040D+00-1.134955793D-01 2.500549799D+00-1.382464681D-06 1.906022991D-09
-1.368396828D-12 4.003528117D-16                 1.095438901D+05 7.538855900D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             6197.428
 1.320690183D+06-4.096048010D+03 7.389101510D+00-2.807751909D-03 7.830991650D-07
-9.310600910D-11 4.016371727D-15                 1.354347306D+05-2.722020908D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             6197.428
 4.101539500D+08-2.538072503D+05 6.239804790D+01-6.542962120D-03 3.507316530D-07
-8.114133770D-12 5.908352630D-17                 2.122867468D+06-5.163550210D+02
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Pb-                Hotop,1985. Gordon,1999.
 3 g 9/97 PB  1.00E   1.00     0.00     0.00     0.00 0  207.2005486      153881.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.776226140D+04 8.235132100D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.776226140D+04 8.235132100D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.776226140D+04 8.235132100D+00
PbBr               Gurvich,1991 pt1 p434 pt2 p360.
 2 tpis91 PB  1.00BR  1.00     0.00     0.00     0.00 0  287.1040000       64821.322
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10146.122
-2.393487988D+03-4.576591210D+01 4.692608280D+00-3.845290630D-04 5.888213500D-07
-4.084792890D-10 1.202515201D-13                 6.662434770D+03 5.991705510D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10146.122
-2.581831670D+06 7.143490760D+03-2.658193640D+00 3.107722260D-03-4.631381540D-07
 1.095529211D-11 1.508555088D-15                -3.970440980D+04 5.959238650D+01
PbBr2              Gurvich,1991 pt1 p437 pt2 p362.
 2 tpis91 PB  1.00BR  2.00     0.00     0.00     0.00 0  367.0080000     -103908.063
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           15021.937
-6.172766360D+03-6.783207630D+01 7.273156140D+00-5.990596120D-04 7.358634610D-07
-4.743604810D-10 1.246922291D-13                -1.427890796D+04-6.987992150D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           15021.937
-1.320421479D+04-1.143074947D+00 7.000972540D+00-4.284471610D-07 1.018044861D-10
-1.234016791D-14 5.971337650D-19                -1.462213750D+04 8.868582650D-01
PbBr3              Gurvich,1991 pt1 p438 pt2 p363.
 2 tpis91 PB  1.00BR  3.00     0.00     0.00     0.00 0  446.9120000     -104010.957
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           19968.643
-1.164424250D+04-1.555151665D+02 1.062317321D+01-1.361947117D-03 1.668738791D-06
-1.073686019D-09 2.818250340D-13                -1.478208304D+04-1.443758579D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           19968.643
-2.787930766D+04-2.633265111D+00 1.000223199D+01-9.807761410D-07 2.326232632D-10
-2.815994460D-14 1.361283735D-18                -1.556981182D+04-1.081765474D+01
PbBr4              Gurvich,1991 pt1 p439 pt2 p364.
 2 tpis91 PB  1.00BR  4.00     0.00     0.00     0.00 0  526.8160000     -182435.511
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           25871.489
-1.176458199D+04-2.567166983D+02 1.402223292D+01-2.224117068D-03 2.716201994D-06
-1.743340164D-09 4.567359750D-13                -2.462125551D+04-2.882020750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           25871.489
-3.880216030D+04-4.382933770D+00 1.300369823D+01-1.620061335D-06 3.834130880D-10
-4.633967180D-14 2.237427066D-18                -2.592327065D+04-2.287710636D+01
PbCL               Gurvich,1991 pt1 p427 pt2 p355.
 2 tpis91 PB  1.00CL  1.00     0.00     0.00     0.00 0  242.6530000       8819.118
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9787.118
-2.902700749D+03-8.293459710D+01 4.714824480D+00-1.931473228D-04 9.105579020D-08
 5.419385230D-11-3.284969700D-14                 1.254460217D+02 4.323194455D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9787.118
-3.854285530D+05 6.922197500D+02 4.509971240D+00-6.853421300D-04 5.087395500D-07
-9.772753810D-11 5.807471580D-15                -5.269684720D+03 6.646491015D+00
PbCL2              Gurvich,1991 pt1 p430 pt2 p357.
 2 tpis91 PB  1.00CL  2.00     0.00     0.00     0.00 0  278.1060000     -175547.471
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           14002.529
 2.830580143D+03-3.134256659D+02 8.212827290D+00-2.585096173D-03 3.109456077D-06
-1.972978208D-09 5.123542480D-13                -2.167569042D+04-9.219412244D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           14002.529
-3.149192744D+04-5.565477580D+00 7.004599540D+00-1.986025455D-06 4.651719590D-10
-5.579137010D-14 2.678143570D-18                -2.327439309D+04-2.140739285D+00
PbCL3              Gurvich,1991 pt1 p432 pt2 p358.
 2 tpis91 PB  1.00CL  3.00     0.00     0.00     0.00 0  313.5590000     -177653.507
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           18255.693
 8.623588970D+02-5.253152750D+02 1.203336337D+01-4.335184980D-03 5.215698350D-06
-3.310022380D-09 8.596970610D-13                -2.180576379D+04-2.694206962D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           18255.693
-5.664412790D+04-9.329514790D+00 1.000771099D+01-3.329727570D-06 7.799330810D-10
-9.354606100D-14 4.490589700D-18                -2.448508643D+04-1.507490870D+01
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PbCL4              Gurvich,1991 pt1 p433 pt2 p359.
 2 tpis91 PB  1.00CL  4.00     0.00     0.00     0.00 0  349.0120000     -327430.362
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23449.438
 1.739405796D+04-8.902139320D+02 1.637565058D+01-7.088992260D-03 8.432567340D-06
-5.305309390D-09 1.368671294D-12                -3.888215620D+04-4.850133784D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23449.438
-8.266679560D+04-1.639486405D+01 1.301336711D+01-5.716141400D-06 1.329368390D-09
-1.585922492D-13 7.581763610D-18                -4.343984220D+04-2.874559263D+01
PbF                Gurvich,1991 pt1 p419 pt2 p350.
 2 tpis91 PB  1.00F   1.00     0.00     0.00     0.00 0  226.1984032      -98867.789
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9268.111
 2.684864255D+04-4.751725640D+02 6.019644370D+00-2.718531008D-03 2.942882954D-06
-1.687543009D-09 4.086122080D-13                -1.079038653D+04-4.983048840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9268.111
-4.734202750D+05 1.027785283D+03 3.888658730D+00-1.649813448D-04 2.931163260D-07
-5.766459650D-11 3.247486190D-15                -2.026165076D+04 9.319483890D+00
PbF2               Gurvich,1991 pt1 p424 pt2 p352.
 2 tpis91 PB  1.00F   2.00     0.00     0.00     0.00 0  245.1968064     -443427.390
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12572.610
 5.920552280D+04-1.052529292D+03 1.028969284D+01-5.876346270D-03 6.102333130D-06
-3.424792640D-09 8.024025420D-13                -4.999050000D+04-2.525115478D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12572.610
-8.505899770D+04-3.074244334D+01 7.023346040D+00-9.455183590D-06 2.108489027D-09
-2.434212002D-13 1.133872429D-17                -5.552236770D+04-5.496073220D+00
PbF3               Gurvich,1991 pt1 p425 pt2 p353.
 2 tpis91 PB  1.00F   3.00     0.00     0.00     0.00 0  264.1952096     -489572.613
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15535.047
 8.553090870D+04-1.731036694D+03 1.556596150D+01-1.022225919D-02 1.089984998D-05
-6.269998820D-09 1.502616508D-12                -5.300335670D+04-5.335733480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15535.047
-1.459704258D+05-4.820396430D+01 1.003685845D+01-1.501095764D-05 3.362474990D-09
-3.896020710D-13 1.820152103D-17                -6.206869590D+04-2.006978661D+01
PbF4               Gurvich,1991 pt1 p426 pt2 p354.
 2 tpis91 PB  1.00F   4.00     0.00     0.00     0.00 0  283.1936128     -799925.173
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19626.227
 1.309963563D+05-2.307299499D+03 1.945201440D+01-1.024522729D-02 9.395874960D-06
-4.626894150D-09 9.450881430D-13                -8.804147460D+04-7.524645820D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19626.227
-2.132616322D+05-8.578621950D+01 1.306428551D+01-2.575563598D-05 5.693324590D-09
-6.526219550D-13 3.022341960D-17                -1.002908979D+05-3.590240280D+01
PbI                Gurvich,1991 pt1 p440 pt2 p365.
 2 tpis91 PB  1.00I   1.00     0.00     0.00     0.00 0  334.1044700      108904.324
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10339.124
-2.717334060D+03-1.542541996D+01 4.565327900D+00-1.061215818D-04 2.414841342D-07
-1.876070301D-10 6.460614270D-14                 1.181864978D+04 7.669802670D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10339.124
-3.901070250D+06 1.147976718D+04-8.176109020D+00 6.523454700D-03-1.522611682D-06
 1.626692202D-10-6.553328880D-15                -6.154433690D+04 9.938404970D+01
PbI2               Gurvich,1991 pt1 p443 pt2 p367.
 2 tpis91 PB  1.00I   2.00     0.00     0.00     0.00 0  461.0089400      -10252.630
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15247.370
-5.904986720D+03-4.833307030D+01 7.195438030D+00-4.298600090D-04 5.291412070D-07
-3.416402820D-10 8.991341920D-14                -3.107780155D+03 1.324773678D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15247.370
-1.088339477D+04-8.164418370D-01 7.000697300D+00-3.079876763D-07 7.331718140D-11
-8.899193880D-15 4.310712500D-19                -3.352096380D+03 2.458605463D+00
PbI3               Gurvich,1991 pt1 p444 pt2 p368.
 2 tpis91 PB  1.00I   3.00     0.00     0.00     0.00 0  587.9134100      21755.412
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21065.012
-1.014996331D+04-5.938078200D+01 1.024073798D+01-5.304694530D-04 6.538623030D-07
-4.225895720D-10 1.113029818D-13                -1.138482403D+02-8.975540500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21065.012
-1.624229573D+04-1.002945584D+00 1.000085839D+01-3.796679740D-07 9.046751720D-11
-1.098840054D-14 5.325388290D-19                -4.138258930D+02-7.579417110D+00
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PbI4                Gurvich,1991 pt1 p445 pt2 p369.
 2 tpis91 PB  1.00I   4.00    0.00    0.00    0.00 0  714.8178800      -41226.459
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27520.541
-1.217096972D+04-7.226317440D+01 1.329294204D+01-6.454660900D-04 7.955761850D-07
-5.141632830D-10 1.354188031D-13                 -8.528148680D+03-2.010457498D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27520.541
-1.958477744D+04-1.223385179D+00 1.300104732D+01-4.633295690D-07 1.104213978D-10
-1.341397771D-14 6.501706110D-19                 -8.893193200D+03-1.840570345D+01
PbO                 Gurvich,1991 pt1 p413 pt2 p345.
 2 tpis91 PB  1.00O   1.00    0.00    0.00    0.00 0  223.1994000       68137.108
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8962.108
 3.424025000D+04-4.198050110D+02 4.720306410D+00 1.451061751D-03-3.206035460D-06
 2.713956273D-09-8.333275610D-13                 9.253186470D+03 4.482891210D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8962.108
 2.426996850D+05-1.107731354D+02 3.180684490D+00 1.991815065D-03-1.079782025D-06
 2.540990941D-10-1.834652493D-14                 8.339391540D+03 1.050920926D+01
PbO2                Gurvich,1991 pt1 p416 pt2 p347.
 2 tpis91 PB  1.00O   2.00    0.00    0.00    0.00 0  239.1988000      136152.734
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12250.934
 7.071058290D+04-1.076757462D+03 9.401711730D+00-1.003861584D-03-1.233815617D-06
 1.858386979D-09-6.834621210D-13                 1.999645981D+04-2.503976748D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12250.934
-1.307796670D+05-7.314361450D+01 7.554083410D+00-2.143421561D-05 4.696464000D-09
-5.344972180D-13 2.460760535D-17                 1.413386101D+04-1.252684909D+01
PbS                 Gurvich,1991 pt1 p448 pt2 p371.
 2 tpis91 PB  1.00S   1.00    0.00    0.00    0.00 0  239.2650000      127945.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9430.113
 1.529840503D+04-3.439746350D+02 5.680630640D+00-2.232931917D-03 2.504608209D-06
-1.470427328D-09 3.577527190D-13                 1.578551202D+04-2.628900926D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9430.113
 2.105441649D+06-5.520413580D+03 9.369249260D+00-1.410262019D-03-1.642683362D-07
 1.451447577D-10-1.393564925D-14                 5.009334530D+04-3.217417657D+01
PbS2                Gurvich,1991 pt1 p450 pt2 p372.
 2 tpis91 PB  1.00S   2.00    0.00    0.00    0.00 0  271.3300000      244049.005
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14021.205
 2.446375880D+04-6.654855460D+02 9.920201180D+00-4.924194380D-03 5.716906290D-06
-3.529488830D-09 8.971138350D-13                 3.044310130D+04-2.295765552D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14021.205
-5.416700300D+04-1.343600342D+01 7.510700360D+00-4.497318630D-06 1.032444494D-09
-1.219580043D-13 5.785804650D-18                 2.701229533D+04-8.714618097D+00
Rb                  Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 1/98 RB  1.00    0.00    0.00    0.00    0.00 0   85.4678000       80900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 1.352856616D+01-2.042232679D-01 2.501213823D+00-3.650619900D-06 5.884722670D-09
-4.842274720D-12 1.596211946D-15                 8.985569210D+03 6.207005480D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-1.138274064D+06 3.804041940D+03-2.750899258D+00 3.891460700D-03-1.632296823D-06
 3.511893140D-10-2.521064422D-14                -1.466454849D+04 4.253442370D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 3.245192200D+08-3.493850870D+05 1.159097652D+02-1.492843123D-02 9.582385060D-07
-2.996233671D-11 3.657332046D-16                 2.636178014D+06-9.586517230D+02
Rb+                 Moore,1971. IP:Moore,1970a. Gordon,1999.
 3 g 1/98 RB  1.00E  -1.00    0.00    0.00    0.00 0   85.4672514      490129.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.820327360D+04 5.520506920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.820327360D+04 5.520506920D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 4.120352830D+07-2.920376515D+04 1.102096776D+01-1.311457972D-03 1.124752629D-07
-5.107819770D-12 9.622794537D-17                 2.850166118D+05-6.672202250D+01
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Rb-                Hotop,1985. Gordon,1999.
 3 g 9/97 RB  1.00E   1.00     0.00     0.00     0.00 0   85.4683486       27818.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.600405796D+03 5.520526170D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.600405796D+03 5.520526170D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.600405796D+03 5.520526170D+00
RbBO2              Gurvich,1982 pt1 p459 pt2 p483.
 2 tpis82 RB  1.00B   1.00O    2.00     0.00     0.00 0  128.2776000     -678977.302
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           14332.698
 4.198657750D+04-6.799448330D+02 8.185151010D+00 2.772536733D-03-6.175770470D-07
-9.426136250D-10 4.722414240D-13                -8.020339590D+04-1.239198887D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           14332.698
 9.154463400D+04-1.668328341D+03 1.117268757D+01-4.505533530D-04 9.681330590D-08
-1.088037652D-11 4.967733660D-16                -7.507903250D+04-3.131951149D+01
RbBr               Gurvich,1982 pt1 p446 pt2 p470.
 2 tpis82 RB  1.00BR  1.00     0.00     0.00     0.00 0  165.3718000     -191510.876
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10319.124
-5.703859700D+03 2.092281597D+01 4.370607370D+00 4.494604780D-04-4.835438840D-07
 3.526068600D-10-9.886538320D-14                -2.449112515D+04 6.427431700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10319.124
 1.609092474D+06-4.466774590D+03 9.064092060D+00-1.995333358D-03 4.016633520D-07
-4.163091400D-12-3.092443341D-15                 4.427467690D+03-2.757714089D+01
RbCL               Gurvich,1982 pt1 p443 pt2 p467.
 2 tpis82 RB  1.00CL  1.00     0.00     0.00     0.00 0  120.9208000     -223322.879
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10057.121
-5.740809580D+03-1.528835285D+01 4.515200900D+00 1.067270745D-04-6.385945590D-09
-1.301381692D-11 1.641459742D-14                -2.814243986D+04 4.190115141D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10057.121
-1.143043004D+06 4.003861880D+03-1.096156782D+00 4.033581280D-03-1.454151464D-06
 2.719263762D-10-1.810463980D-14                -5.297686040D+04 4.311317822D+01
RbF                Gurvich,1982 pt1 p440 pt2 p464.
 2 tpis82 RB  1.00F   1.00     0.00     0.00     0.00 0  104.4662032     -333511.885
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9588.115
 3.287360190D+04-6.080907460D+02 7.406622360D+00-7.277864720D-03 1.013930727D-05
-7.141372500D-09 2.014332982D-12                -3.849834130D+04-1.375750778D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9588.115
-8.544811150D+05 2.633756505D+03 1.216216506D+00 2.136494067D-03-6.728426080D-07
 1.134905135D-10-6.825624440D-15                -5.810179110D+04 2.588118896D+01
RbH                Gurvich,1982 pt1 p435 pt2 p459.
 2 tpis82 RB  1.00H   1.00     0.00     0.00     0.00 0   86.4757400      119324.106
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8820.106
 8.908270610D+03 4.649870400D+01 1.833967623D+00 8.444279140D-03-1.167538647D-05
 8.010389420D-09-2.162578321D-12                 1.328248009D+04 1.279544976D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8820.106
-2.937703530D+06 9.379817260D+03-7.542563460D+00 7.493226800D-03-2.159228887D-06
 2.871300173D-10-1.459981256D-14                -4.595518830D+04 8.365664320D+01
RbI                Gurvich,1982 pt1 p449 pt2 p473.
 2 tpis82 RB  1.00I   1.00     0.00     0.00     0.00 0  212.3722700     -138480.874
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10459.126
-7.693052800D+02-2.968608844D+01 4.648745840D+00-2.962415236D-04 5.978135340D-07
-4.351255250D-10 1.313617336D-13                -1.786610717D+04 5.812409830D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10459.126
 4.297424850D+06-1.296911161D+04 1.958730402D+01-8.458425590D-03 2.463480035D-06
-3.191575730D-10 1.458455589D-14                 6.432948040D+04-1.009499336D+02
RbK                Gurvich,1982 pt1 p462 pt2 p486.
 2 tpis82 RB  1.00K   1.00     0.00     0.00     0.00 0  124.5661000      120013.330
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10808.130
 2.494695429D+04-4.553060660D+02 7.686189950D+00-1.108112244D-02 2.093398586D-05
-1.824445366D-08 5.617645360D-12                 1.516136160D+04-1.063563675D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10808.130
-4.175391070D+06 5.918588510D+03 9.202649420D+00-1.060933600D-02 4.964826060D-06
-8.716698790D-10 5.221887960D-14                -3.272769040D+04-1.372401997D+01
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RbLi              Gurvich,1982 pt1 p460 pt2 p484.
 2 tpis82 RB  1.00LI  1.00    0.00    0.00    0.00 0   92.4088000     164181.324
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10276.124
-2.263413044D+03-2.888496910D+01 4.555826540D+00 3.625667530D-04-9.598002220D-07
 1.631010244D-09-8.159825980D-13                  1.853455250D+04 2.831743182D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10276.124
 1.085515194D+07-3.805106970D+04 5.516555040D+01-3.128845612D-02 9.261650250D-06
-1.264671408D-09 6.431662050D-14                  2.543964131D+05-3.520758710D+02
RbNO2             Gurvich,1982 pt1 p454 pt2 p478.
 2 tpis82 RB  1.00N   1.00O   2.00    0.00    0.00 0  131.4733000    -187629.777
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15770.223
-7.199420030D+04 1.265802595D+03-2.415715742D+00 3.054641420D-02-3.684004050D-05
 2.247716481D-08-5.547527430D-12                 -3.037381667D+04 4.814256904D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15770.223
-1.644994453D+05-8.499443440D+02 1.063080575D+01-2.517893988D-04 5.561420120D-08
-6.378805600D-12 2.957679896D-16                 -2.128590982D+04-2.568367325D+01
RbNO3             Gurvich,1982 pt1 p456 pt2 p480.
 2 tpis82 RB  1.00N   1.00O   3.00    0.00    0.00 0  147.4727000    -314972.483
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16367.517
-2.664669172D+04 8.807634790D+02-3.159459457D+00 4.271229020D-02-5.351029210D-05
 3.360969750D-08-8.503290510D-12                 -4.353595460D+04 4.943052899D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16367.517
-3.147413867D+05-1.371457846D+03 1.401319759D+01-4.030275020D-04 8.878332290D-08
-1.016221214D-11 4.704254090D-16                 -3.504339940D+04-4.619379241D+01
RbNa              Gurvich,1982 pt1 p461 pt2 p485.
 2 tpis82 RB  1.00NA  1.00    0.00    0.00    0.00 0  108.4575700     131470.328
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10665.128
 2.974455567D+04-5.082790590D+02 7.734033520D+00-1.013006840D-02 1.745455325D-05
-1.398725470D-08 3.968106770D-12                  1.682379436D+04-1.240085290D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10665.128
 4.297114270D+06-1.831013588D+04 3.454394200D+01-2.230134993D-02 7.339874530D-06
-1.064784996D-09 5.617598460D-14                  1.242610951D+05-1.993661980D+02
RbO               Gurvich,1982 pt1 p429 pt2 p452.
 2 tpis82 RB  1.00O   1.00    0.00    0.00    0.00 0  101.4672000      52489.324
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10337.124
 1.900081316D+05-3.428228990D+03 2.480251273D+01-5.051654580D-02 6.476338760D-05
-4.198012420D-08 1.093889043D-11                  2.083898450D+04-1.097559150D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10337.124
 6.170756880D+05-2.175089620D+03 8.290412210D+00-2.996487663D-03 1.233144275D-06
-2.115810631D-10 1.242607430D-14                  1.828164827D+04-2.117386042D+01
RbOH              Gurvich,1997.
 2 g 9/97 RB  1.00O   1.00H   1.00    0.00    0.00 0  102.4751400    -238000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11761.202
 1.213832721D+04-5.441411590D+02 8.459814640D+00-3.561526560D-03 2.992872390D-06
-7.280267400D-10-4.553847180D-14                 -2.787262486D+04-1.913421991D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11761.202
 8.958583130D+05-2.332339000D+03 7.971192480D+00 1.044439355D-04-6.328257750D-08
 1.029358824D-11-5.743277790D-16                 -1.515568947D+04-1.950051629D+01
Rb2Br2            Gurvich,1982 pt1 p447 pt2 p471.
 2 tpis82 RB  2.00BR  2.00    0.00    0.00    0.00 0  330.7436000    -551801.433
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21696.566
-8.005525400D+03-2.111968088D+01 1.008629404D+01-1.911936090D-04 2.366059490D-07
-1.533722380D-10 4.048725060D-14                 -6.927313600D+04-9.622434630D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21696.566
-1.014535336D+04-3.601550320D-01 1.000031058D+01-1.380745805D-07 3.302067950D-11
-4.021581820D-15 1.953006729D-19                 -6.937960880D+04-9.122562360D+00
Rb2CL2            Gurvich,1982 pt1 p444 pt2 p468.
 2 tpis82 RB  2.00CL  2.00    0.00    0.00    0.00 0  241.8416000    -618373.536
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20785.574
-1.125039522D+04-6.756953990D+01 1.027381915D+01-6.031848990D-04 7.433324780D-07
-4.803372160D-10 1.264973638D-13                 -7.706757500D+04-1.363652575D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20785.574
-1.818875133D+04-1.137903580D+00 1.000097318D+01-4.302156400D-07 1.024725787D-10
-1.244291058D-14 6.028912390D-19                 -7.740897670D+04-1.204843385D+01
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Rb2F2              Gurvich,1982 pt1 p441 pt2 p465.
 2 tpis82 RB  2.00F   2.00    0.00    0.00    0.00 0  208.9324064    -854913.348
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18889.758
-8.178347100D+03-3.334733540D+02 1.131540799D+01-2.842914926D-03 3.454959580D-06
-2.209373419D-09 5.772073270D-13                -1.042230504D+05-2.368991587D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18889.758
-4.376574390D+04-5.761452040D+00 1.000482691D+01-2.104159548D-06 4.962416270D-10
-5.982174970D-14 2.882751742D-18                -1.059176154D+05-1.603254014D+01
Rb2I2              Gurvich,1982 pt1 p450 pt2 p474.
 2 tpis82 RB  2.00I   2.00    0.00    0.00    0.00 0  424.7445400    -432956.482
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22217.518
-5.839663550D+03-9.527537900D+00 1.003904495D+01-8.668754000D-05 1.074384368D-07
-6.972122230D-11 1.842065721D-14                -5.502780960D+04-7.174113320D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22217.518
-6.799834640D+03-1.642527699D-01 1.000014200D+01-6.321420730D-08 1.512811170D-11
-1.843027189D-15 8.951244180D-20                -5.507579620D+04-6.948045390D+00
Rb2O               Gurvich,1982 pt1 p431 pt2 p455.
 2 tpis82 RB  2.00O   1.00    0.00    0.00    0.00 0  186.9350000    -108929.421
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14215.779
 1.971276138D+04-4.627508860D+02 8.588293130D+00-3.085559728D-03 3.451980140D-06
-2.068570368D-09 5.132480500D-13                -1.284854711D+04-1.264891828D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14215.779
-3.846360090D+04-1.082831019D+01 7.008421890D+00-3.476228120D-06 7.869785060D-10
-9.195683850D-14 4.325201520D-18                -1.525373768D+04-3.230388780D+00
Rb2O2              Gurvich,1982 pt1 p434 pt2 p457.
 2 tpis82 RB  2.00O   2.00    0.00    0.00    0.00 0  202.9344000    -215848.468
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16847.132
 3.260553230D+04-7.578164720D+02 1.070815124D+01 1.148004329D-03-3.291243670D-06
 2.853106637D-09-8.721590680D-13                -2.475317258D+04-2.434276460D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16847.132
-1.318567396D+05-9.647737790D+01 1.007222726D+01-2.894921706D-05 6.405639100D-09
-7.351419390D-13 3.408561710D-17                -2.882179733D+04-1.910948823D+01
Rb2O2H2            Gurvich,1997.  .
 2 g 9/97 RB  2.00O   2.00H   2.00    0.00    0.00 0  204.9502800    -639000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23407.379
-4.577076530D+03-8.417631000D+02 1.704083828D+01-5.357882540D-03 3.951778770D-06
-2.051775094D-10-4.085416910D-13                -7.694982170D+04-5.435412780D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23407.379
 1.792711652D+06-4.659406600D+03 1.693822422D+01 2.106246492D-04-1.269617470D-07
 2.063382927D-11-1.150861507D-15                -5.024117630D+04-6.027054920D+01
Rb2SO4             Gurvich,1982 pt1 p452 pt2 p476.
 2 g10/99 RB  2.00S   1.00O   4.00    0.00    0.00 0  266.9982000   -1096592.052
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23321.948
 6.094854930D+04-6.889705900D+02 7.034242180D+00 3.933945470D-02-5.498920510D-05
 3.716341080D-08-9.919863380D-12                -1.311877657D+05-4.450168488D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23321.948
-5.302898310D+05-9.515435450D+02 1.971013517D+01-2.842916301D-04 6.289142940D-08
-7.219324300D-12 3.348718190D-16                -1.338713151D+05-7.056246882D+01
Rn                 Ref-Elm. Moore,1971. Gordon,1999.
 3 g 5/97 RN  1.00    0.00    0.00    0.00    0.00 0  222.0176000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 3.389432090D-06-1.311675533D-07 2.500000001D+00-2.978593139D-12 4.337050730D-15
-3.182040220D-18 9.247787030D-22                -7.453749990D+02 6.952441980D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 2.730190029D+04-8.284672620D+01 2.598178483D+00-5.813729850D-05 1.819136527D-08
-2.866656182D-12 1.789322176D-16                -2.202809340D+02 6.255005710D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 9.180866680D+08-6.245854600D+05 1.724946531D+02-2.325758595D-02 1.636222413D-06
-5.369173150D-11 6.507189926D-16                 4.883105900D+06-1.449516146D+03
Rn+                Moore,1971. Gordon,1999.
 3 g 1/97 RN  1.00E  -1.00    0.00    0.00    0.00 0  222.0170514    1043270.264
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-9.697148970D-02 1.106742047D-03 2.499994937D+00 1.189388239D-08-1.515895754D-11
 9.958934810D-15-2.640751817D-18                 1.247304760D+05 8.338761700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-1.998285319D+04 5.930675660D+01 2.432476003D+00 3.716025920D-05-1.012057848D-08
 1.192256661D-12-3.184521980D-17                 1.243528478D+05 8.821997790D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-2.408821471D+07 1.571151698D+04-1.411683762D+00 4.495267600D-04-2.324033616D-08
 5.830243350D-13-5.821682810D-18                 9.187457500D+02 4.233613280D+01
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Appendix D (*continued*)

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S                Hf: Cox,1989 p22. Martin,1990. Gordon,1999.
 3 g 5/97 S   1.00    0.00    0.00    0.00    0.00 0   32.0650000     277170.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6657.425
-3.174841820D+02-1.924704923D+02 4.686825930D+00-5.841365600D-03 7.538533520D-06
-4.863586040D-09 1.256976992D-12                 3.323592180D+04-5.718523969D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6657.425
-4.854244790D+05 1.438830408D+03 1.258504116D+00 3.797990430D-04 1.630685864D-09
-9.547095850D-12 8.041466646D-16                 2.334995270D+04 1.559554855D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6657.425
-1.302005414D+08 6.909362020D+04-1.176228025D+01 1.601540850D-03-1.050533340D-07
 4.341829020D-12-7.675621927D-17                -5.261485030D+05 1.322195251D+02
S+               Martin,1990. Gordon,1999.
 3 g 1/98 S   1.00E  -1.00    0.00    0.00    0.00 0   32.0644514    1282496.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.535026117D+05 5.436223340D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.346218684D+06-4.056871510D+03 7.153436550D+00-2.523562352D-03 6.429539610D-07
-6.431672160D-11 2.141387919D-15                 1.792823835D+05-2.786935079D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.542254583D+08-1.023073546D+05 2.591796942D+01-2.111469141D-03 9.215571560D-08
-1.964168821D-12 2.096218597D-17                 9.622418410D+05-2.017239957D+02
S-               Hotop,1985. Gordon,1999.
 3 g 4/97 S   1.00E   1.00    0.00    0.00    0.00 0   32.0655486      70368.505
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6464.905
-2.596051473D+03-1.422398653D+02 4.007825670D+00-3.608855910D-03 4.236230000D-06
-2.520987604D-09 6.079479760D-13                 8.197793070D+03-2.582377345D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6464.905
 2.730311692D+03 1.414072078D+02 2.403340775D+00 3.693577530D-05-7.944080440D-09
 8.952208380D-13-4.099662820D-17                 6.931195700D+03 6.574986902D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6464.905
-1.223682088D+05 1.203125842D+02 2.473942293D+00 2.935459895D-06-1.808577869D-10
 5.778854260D-15-7.490337240D-20                 6.947841220D+03 6.070579772D+00
SCL              Chase,1998 p803.
 2 j 6/78 S   1.00CL  1.00    0.00    0.00    0.00 0   67.5180000     156465.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9819.151
 1.613051454D+04-5.606249550D+02 8.064931130D+00-9.186326400D-03 1.224205395D-05
-8.209562020D-09 2.205087197D-12                 1.997739280D+04-1.693354410D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9819.151
-9.405123450D+04 3.629760850D+02 4.069959360D+00 3.034029742D-04-8.248301390D-08
 1.252700734D-11-6.417463650D-16                 1.523111069D+04 6.014528409D+00
SCL2             Chase,1998 p856.
 2 j 6/78 S   1.00CL  2.00    0.00    0.00    0.00 0  102.9710000     -17573.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12445.325
 5.792311830D+04-1.062447681D+03 1.037694738D+01-6.130229020D-03 6.463486000D-06
-3.679038050D-09 8.731931650D-13                 1.262475821D+03-2.691769492D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12445.325
-2.341039963D+05 4.287569580D+02 6.471415390D+00 3.179476740D-04-9.747483080D-08
 1.393318570D-11-6.394795170D-16                -7.210473700D+03-2.774273151D+00
SCL2+            Chase,1998 p857.
 3 j 6/78 S   1.00CL  2.00E  -1.00    0.00    0.00 0  102.9704514     901383.347
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12453.247
 4.934876870D+04-9.601641020D+02 9.884792780D+00-4.950257170D-03 4.946286970D-06
-2.678720604D-09 6.076844030D-13                 1.112812037D+05-2.342664942D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12453.247
-2.339403605D+05 5.516283260D+02 6.125212160D+00 6.771056320D-04-2.674382769D-07
 4.935938880D-11-2.955831247D-15                 1.026787381D+05 1.365611954D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12453.247
 1.159729818D+08-4.231290230D+04 7.753324790D+00 1.215229138D-03-1.338847939D-07
 5.496166430D-12-8.098916920D-17                 4.756171550D+05-2.296333258D+01
SD               Chase,1998 p1039.
 2 j 6/77 S   1.00D   1.00    0.00    0.00    0.00 0   34.0791020     138490.892
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9294.443
-3.295574990D+04 1.647104687D+02 4.978984550D+00-8.031585710D-03 1.653766397D-05
-1.345197981D-08 4.000431530D-12                 1.435862329D+04-1.997334017D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9294.443
 2.456732490D+05-1.180034105D+03 5.284690050D+00-2.384319882D-04 6.009960290D-08
-7.131163640D-12 4.035858700D-16                 2.265545124D+04-8.350483655D+00
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Appendix D (*continued*)

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SF                Gurvich,1989 pt1 p302 pt2 p183.
 2 tpis89 S   1.00F   1.00    0.00    0.00    0.00 0   51.0634032      15445.561
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9470.114
 1.206456774D+04-2.910270770D+02 5.480101570D+00-1.975880235D-03 2.473685990D-06
-1.610904623D-09 4.310038540D-13                 1.991337574D+03-4.544138975D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9470.114
 7.634580750D+05-2.423638430D+03 7.352198710D+00-1.598026079D-03 4.868515020D-07
-6.478000530D-11 2.980297310D-15                 1.577461591D+04-1.902584835D+01
SF+               Chase,1998 p1091 6/76.
 3 g 1/01 S   1.00F   1.00E  -1.00    0.00    0.00 0   51.0628546     994570.218
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8864.318
 6.578303670D+04-6.986699970D+02 5.621292240D+00-6.909274110D-04-1.282392780D-07
 4.021320420D-10-1.424033453D-13                 1.221751247D+05-6.682377715D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8864.318
-9.374943900D+05 2.377214240D+03 2.052929113D+00 1.081609837D-03-1.535468024D-07
 8.222691900D-12 3.259746880D-17                 1.026849122D+05 1.887705768D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8864.318
-4.833080340D+07 3.315103280D+04-4.246678200D+00 1.269355284D-03-7.864010490D-08
 2.406680266D-12-2.892795916D-17                -1.419262455D+05 7.611520762D+01
SF-               Gurvich,1989 pt1 p304 pt2 p184.
 2 tpis89 S   1.00F   1.00E   1.00    0.00    0.00 0   51.0639518     -231346.893
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8875.107
 5.019879280D+04-5.321549310D+02 4.904849010D+00 9.915307420D-04-2.270841545D-06
 1.844749756D-09-5.357057200D-13                -2.611388646D+04-3.637468065D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8875.107
 2.068923125D+05-1.324372811D+03 6.646211240D+00-1.641781588D-03 6.783883120D-07
-1.198331099D-10 7.121739540D-15                -2.150994816D+04-1.470239183D+01
SF2               Gurvich,1989 pt1 p305 pt2 p185.
 2 tpis89 S   1.00F   2.00    0.00    0.00    0.00 0   70.0618064     -293188.734
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11048.373
 6.870871130D+04-8.432418250D+02 6.269496400D+00 6.484142450D-03-1.145126533D-05
 8.770291560D-09-2.542611601D-12                -3.229980700D+04-8.800025780D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11048.373
-1.702612287D+05-1.497038204D+02 7.110934140D+00-4.407741600D-05 9.682208310D-09
-1.104468959D-12 5.095308780D-17                -3.704289490D+04-1.095253960D+01
SF2+              Chase,1998 p1144 12/76.
 3 g 1/01 S   1.00F   2.00E  -1.00    0.00    0.00 0   70.0612578     706015.901
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11234.180
 1.311648923D+05-1.552127914D+03 9.803424720D+00-2.488118587D-03 7.501565130D-07
 3.135384495D-10-1.986281446D-13                 9.137758390D+04-2.792300566D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11234.180
-3.847531020D+05 5.327893020D+02 6.281908900D+00 4.522790120D-04-1.426421096D-07
 2.079708115D-11-9.691709890D-16                 7.884213810D+04-4.216110530D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11234.180
-1.635869714D+08 1.203460697D+05-2.737707929D+01 4.676205400D-03-3.035589058D-07
 9.547077170D-12-1.181291324D-16                -8.508449070D+05 2.843901430D+02
SF2-              Chase,1998 p1145 12/76.
 3 g 1/01 S   1.00F   2.00E   1.00    0.00    0.00 0   70.0623550     -394794.960
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12124.875
 5.284572480D+04-1.032342905D+03 1.006404631D+01-5.209503250D-03 5.168381370D-06
-2.783420867D-09 6.286410080D-13                -4.423303780D+04-2.699266970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12124.875
-9.376618950D+04-3.638995270D+01 7.027942820D+00-1.142143365D-05 2.566295898D-09
-2.981125977D-13 1.395700722D-17                -4.967050330D+04-8.483087899D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12124.875
-2.168882121D+04-5.051042570D+01 7.011106220D+00-1.262936151D-06 7.835542760D-11
-2.517641418D-15 3.278401810D-20                -4.951246860D+04-8.370909449D+00
SF3               Gurvich,1989 pt1 p306 pt2 p186.
 2 tpis89 S   1.00F   3.00    0.00    0.00    0.00 0   89.0602096     -504101.395
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13548.265
 1.284008253D+05-2.084871223D+03 1.423421102D+01-4.015032190D-03 9.152258040D-07
 1.109809721D-09-5.988602720D-13                -5.239517340D+04-5.187194724D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13548.265
-2.411283460D+05-1.418950375D+02 1.010590548D+01-4.231526910D-05 9.336120600D-09
-1.068727665D-12 4.944342600D-17                -6.358445860D+04-2.489561796D+01
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SF3+              Chase,1998 p1170.
 3 j12/76 S   1.00F   3.00E  -1.00    0.00    0.00 0   89.0596610     393583.476
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12409.148
 2.157633857D+05-2.564488498D+03 1.323216044D+01-1.749580869D-04-3.712958710D-06
 3.580688420D-09-1.084376153D-12                 5.876088420D+04-5.024130184D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12409.148
-3.778260750D+05-1.621770252D+02 9.960265970D+00 1.237729568D-04-6.442207890D-08
 1.300856025D-11-7.915106980D-16                 4.415426810D+04-2.673900770D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12409.148
 8.358347800D+06 2.002176210D+03 7.115714750D+00 6.563028420D-04-5.120344380D-08
 1.781530495D-12-2.365386482D-17                 3.575488850D+04-4.384285323D+00
SF3-              Gurvich,1989 pt1 p307 pt2 p187.
 2 tpis89 S   1.00F   3.00E   1.00    0.00    0.00 0   89.0607582    -790124.207
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13722.893
 1.546500675D+05-2.469768526D+03 1.657548496D+01-1.020137434D-02 9.368008460D-06
-4.725672600D-09 1.009661431D-12                -8.500157900D+04-6.532166474D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13722.893
-2.253860964D+05-1.308890242D+02 1.009972380D+01-4.052345530D-05 9.064565220D-09
-1.049320641D-12 4.899201260D-17                -9.800227200D+04-2.524368023D+01
SF4               Gurvich,1989 pt1 p307 pt2 p188.
 2 tpis89 S   1.00F   4.00    0.00    0.00    0.00 0  108.0586128    -760000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15382.882
 1.636183265D+05-2.531316261D+03 1.559106568D+01 3.326704310D-03-1.054935525D-05
 9.391363050D-09-2.914816694D-12                -8.115558920D+04-6.131532958D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15382.882
-3.777125160D+05-2.937595659D+02 1.321902007D+01-8.747669450D-05 1.929905265D-08
-2.209423506D-12 1.022335559D-16                -9.483175340D+04-4.243061278D+01
SF4+              Chase,1998 p1188.
 3 j12/76 S   1.00F   4.00E  -1.00    0.00    0.00 0  108.0580642     416111.962
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16505.547
 2.309587324D+05-3.383777670D+03 2.101756367D+01-1.106529555D-02 9.038097280D-06
-4.055912640D-09 7.712575180D-13                 6.425375150D+04-8.938224908D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16505.547
-4.189172750D+05 4.002889640D+01 1.283873264D+01 1.340235036D-04-4.818135180D-08
 7.574595960D-12-3.696670780D-16                 4.469944230D+04-3.760378598D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16505.547
-3.761690270D+07 2.881726011D+04 4.470948840D+00 1.170801362D-03-7.325658000D-08
 2.214151827D-12-2.649348632D-17                -1.772949712D+05 3.397688982D+01
SF4-              Chase,1998 p1189.
 3 j12/76 S   1.00F   4.00E   1.00    0.00    0.00 0  108.0591614    -887464.320
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18480.321
 1.005523355D+05-2.267351994D+03 1.979284560D+01-1.163761842D-02 1.161792139D-05
-6.288895470D-09 1.426371272D-12                -9.895597430D+04-7.916366078D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18480.321
 3.208822080D+05-1.710416599D+03 1.494425485D+01-1.057207329D-03 2.742846920D-07
-2.905761211D-11 1.084482543D-15                -1.005231225D+05-5.164256578D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18480.321
 5.436095670D+07-3.546125020D+04 2.105391090D+01-7.366819310D-04 3.537247530D-08
-8.825254090D-13 9.049180280D-18                 1.694175033D+05-1.089710894D+02
SF5               Gurvich,1989 pt1 p308 pt2 p189.
 2 tpis89 S   1.00F   5.00    0.00    0.00    0.00 0  127.0570160    -902663.287
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18811.479
 2.224176850D+05-4.043991750D+03 2.707196786D+01-1.744176604D-02 1.604198715D-05
-7.997243020D-09 1.667968061D-12                -9.220078270D+04-1.232426279D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18811.479
-3.892426370D+05-1.825826536D+02 1.613765057D+01-5.544834230D-05 1.231433706D-08
-1.417173409D-12 6.584889400D-17                -1.135671054D+05-5.577524201D+01
SF5+              Chase,1998 p1200.
 3 j12/77 S   1.00F   5.00E  -1.00    0.00    0.00 0  127.0564674     172644.006
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16347.344
 3.777135620D+05-5.646075120D+03 3.049404270D+01-2.176488368D-02 1.941993792D-05
-9.556201140D-09 2.000077302D-12                 4.592204810D+04-1.489889627D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16347.344
-9.814342320D+05 7.208817390D+02 1.564386818D+01-2.452519972D-04 2.241690996D-07
-3.990035890D-11 2.279087545D-15                 9.090953190D+03-5.531460631D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16347.344
 9.063623020D+06-8.079630910D+03 1.805068495D+01-2.624346278D-05-4.739171840D-09
 2.144486076D-13-2.737984333D-18                 7.597515770D+04-7.692263871D+01
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SF5-              Gurvich,1989 pt1 p309 pt2 p190.
 2 tpis89 S   1.00F   5.00E   1.00    0.00    0.00 0  127.0575646   -1204622.287
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19049.913
 2.095031134D+05-3.930081140D+03 2.702127215D+01-1.792973203D-02 1.718122152D-05
-9.000560190D-09 1.988018147D-12                -1.291816581D+05-1.231672857D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19049.913
-3.733219200D+05-1.793729521D+02 1.613699748D+01-5.577539970D-05 1.249477046D-08
-1.448104799D-12 6.767462300D-17                -1.498554401D+05-5.631439391D+01
SF6               Gurvich,1989 pt1 p311 pt2 p191.
 2 tpis89 S   1.00F   6.00    0.00    0.00    0.00 0  146.0554192   -1219400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16940.067
 3.309526740D+05-4.737685050D+03 2.247738068D+01 1.046954309D-02-2.560641961D-05
 2.153716967D-08-6.516098960D-12                -1.255360583D+05-1.091760145D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16940.067
-7.306726500D+05-6.367056550D+02 1.947442853D+01-1.894325671D-04 4.178722830D-08
-4.783744950D-12 2.213516129D-16                -1.510609837D+05-8.147574587D+01
SF6-              Chase,1998 p1206.
 3 j 6/77 S   1.00F   6.00E   1.00    0.00    0.00 0  146.0559678   -1341876.033
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17490.714
 4.985809210D+05-6.934445740D+03 3.441318330D+01-1.984032360D-02 1.497871222D-05
-6.133234650D-09 1.045159581D-12                -1.297069066D+05-1.747984495D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17490.714
-6.818073510D+05-5.947429960D+02 1.945009842D+01-1.820212649D-04 4.057079570D-08
-4.683820930D-12 2.182263999D-16                -1.658902452D+05-7.965845887D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17490.714
 1.777074958D+05-6.533730340D+02 1.914322537D+01-1.624883879D-05 1.006454127D-09
-3.230395820D-14 4.203897370D-19                -1.646993323D+05-7.753346267D+01
SH                D0:Continetti,1991. Gurvich,1989 pt1 p296 pt2 p179.
 2 g10/01 S   1.00H   1.00    0.00    0.00    0.00 0   33.0729400     142135.309
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9098.109
 6.389434680D+03-3.747960920D+02 7.548145770D+00-1.288875477D-02 1.907786343D-05
-1.265033728D-08 3.235158690D-12                 1.742902395D+04-1.760761843D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9098.109
 1.682631601D+06-5.177152210D+03 9.198168520D+00-2.323550224D-03 6.543914780D-07
-8.468470420D-11 3.864741550D-15                 4.899214490D+04-3.770400275D+01
SH-               Gurvich,1989 pt1 p297 pt2 p180.
 2 g10/01 S   1.00H   1.00E   1.00    0.00    0.00 0   33.0734886     -86574.096
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8646.104
 3.878070760D+04-5.742590600D+02 6.898544460D+00-1.001352412D-02 1.486460572D-05
-9.750368900D-09 2.446909813D-12                -8.735388980D+03-1.615966489D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8646.104
 1.198715402D+06-3.894846820D+03 7.660422330D+00-1.355237590D-03 3.342370240D-07
-3.350722310D-11 9.055084780D-16                 1.317477387D+04-2.818370616D+01
SN                Gurvich,1989 pt1 p392 pt2 p252.
 2 tpis89 S   1.00N   1.00    0.00    0.00    0.00 0   46.0717000     267388.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9393.113
-6.835412350D+04 1.147567483D+03-2.877802574D+00 1.724864320D-02-2.058999904D-05
 1.261369640D-08-3.139030141D-12                 2.564143612D+04 4.224006964D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9393.113
-4.837284460D+05 1.058075590D+03 3.086198804D+00 9.111360780D-04-2.764061722D-07
 4.157370110D-11-2.128351755D-15                 2.379345477D+04 1.033222139D+01
SO                Gurvich,1989 pt1 p286 pt2 p173.
 2 tpis89 S   1.00O   1.00    0.00    0.00    0.00 0   48.0644000       4760.306
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8798.106
-3.342757000D+04 6.403862500D+02-1.006641228D+00 1.381512705D-02-1.704486364D-05
 1.061294930D-08-2.645796205D-12                -3.371292190D+03 3.093861963D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8798.106
-1.443410557D+06 4.113874360D+03-5.383695780D-01 2.794153269D-03-6.633352260D-07
 7.838221190D-11-3.560509070D-15                -2.708838059D+04 3.615358329D+01
SO-               Gurvich,1989 pt1 p288 pt2 p174.
 2 tpis89 S   1.00O   1.00E   1.00    0.00    0.00 0   48.0649486     -105968.086
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9467.114
 8.420196970D+03-6.916586680D+01 3.837666610D+00 2.166482062D-03-2.811222562D-06
 1.793426453D-09-4.521795950D-13                -1.354162531D+04 4.316141603D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9467.114
 1.767156147D+05-6.633987360D+02 5.177279810D+00-2.853461125D-04 7.214421530D-08
-3.676469490D-12-2.910092894D-16                -9.984438010D+03-3.951456757D+00
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SOF2              Gurvich,1989 pt1 p312 pt2 p192.
 2 tpis89 S   1.000   1.00F   2.00    0.00    0.00 0   86.0612064    -584952.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12624.845
 6.114579650D+04-9.081119670D+02 6.883623260D+00 1.192459695D-02-1.671006410D-05
 1.110723646D-08-2.910788226D-12                -6.742935840D+04-1.125458745D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12624.845
-2.510555779D+05-6.074439610D+02 1.045046709D+01-1.796384979D-04 3.964169730D-08
-4.543055240D-12 2.104969923D-16                -7.072071710D+04-2.904334504D+01
SO2               Gurvich,1989 pt1 p288 pt2 p175.
 2 tpis89 S   1.000   2.00    0.00    0.00    0.00 0   64.0638000    -296810.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10548.127
-5.310842140D+04 9.090311670D+02-2.356891244D+00 2.204449885D-02-2.510781471D-05
 1.446300484D-08-3.369070940D-12                -4.113752080D+04 4.045512519D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10548.127
-1.127640116D+05-8.252261380D+02 7.616178630D+00-1.999327610D-04 5.655631430D-08
-5.454316610D-12 2.918294102D-16                -3.351308690D+04-1.655776085D+01
SO2-              Gurvich,1989 pt1 p290 pt2 p176.
 2 tpis89 S   1.000   2.00E   1.00    0.00    0.00 0   64.0643486    -408606.069
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10749.431
 9.460901660D+04-8.562691050D+02 5.360074220D+00 7.609576740D-03-1.092005659D-05
 7.202547730D-09-1.850138220D-12                -4.580094810D+04-3.929956604D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10749.431
-1.793400005D+05-3.663168760D+02 7.274441050D+00-1.101944663D-04 2.443328132D-08
-2.809735019D-12 1.305160431D-16                -4.973072610D+04-1.261421156D+01
SO2CL2            Chase,1998 p847.
 2 j 6/71 S   1.000   2.00CL  2.00    0.00    0.00 0  134.9698000    -354803.200
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16028.704
 6.821592390D+03-5.849569200D+02 8.596756910D+00 1.197228675D-02-1.333760700D-05
 7.126129000D-09-1.496150016D-12                -4.230783810D+04-1.652458363D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16028.704
-2.376639109D+05-9.647740410D+02 1.371469904D+01-2.850327057D-04 6.293509620D-08
-7.217844260D-12 3.346840220D-16                -4.190072990D+04-4.481942575D+01
SO2FCL            Chase,1998 p754.
 2 j 6/71 S   1.000   2.00F   1.00CL  1.00    0.00 0  118.5152032    -556472.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14700.981
 3.684561300D+04-8.038358950D+02 7.526186880D+00 1.620141782D-02-1.970595270D-05
 1.166250330D-08-2.759241465D-12                -6.503598190D+04-1.299745646D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14700.981
-2.915402438D+05-1.107134423D+03 1.381845158D+01-3.258514460D-04 7.184741000D-08
-8.230625200D-12 3.812925620D-16                -6.552472690D+04-4.709166446D+01
SO2F2             Gurvich,1989 pt1 p313 pt2 p193.
 2 tpis89 S   1.000   2.00F   2.00    0.00    0.00 0  102.0606064    -760000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13490.451
 5.533153530D+04-8.074639680D+02 5.287172160D+00 2.294547775D-02-2.891025299D-05
 1.785631907D-08-4.418919500D-12                -8.899428820D+04-4.124256607D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13490.451
-3.403904450D+05-1.309288764D+03 1.396601541D+01-3.840088150D-04 8.456688780D-08
-9.678246870D-12 4.480014280D-16                -8.901994140D+04-5.109270050D+01
SO3               Gurvich,1989 pt1 p292 pt2 p177.
 2 tpis89 S   1.000   3.00    0.00    0.00    0.00 0   80.0632000    -395900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11688.499
-3.952855290D+04 6.208572570D+02-1.437731716D+00 2.764126467D-02-3.144958662D-05
 1.792798000D-08-4.126386660D-12                -5.184106170D+04 3.391331216D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11688.499
-2.166923781D+05-1.301022399D+03 1.096287985D+01-3.837100020D-04 8.466889040D-08
-9.705399290D-12 4.498397540D-16                -4.398283990D+04-3.655217314D+01
S2                Gurvich,1989 pt1 p270 pt2 p165.
 2 tpis89 S   2.00    0.00    0.00    0.00    0.00 0   64.1300000     128600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9132.110
 3.528091780D+04-4.222156580D+02 4.677433490D+00 1.724046361D-03-3.862208210D-06
 3.336156340D-09-9.930661540D-13                 1.654767715D+04-7.957279032D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9132.110
-1.588128788D+04 6.315480880D+02 2.449628069D+00 1.986240565D-03-6.507927240D-07
 1.002813651D-10-5.596990050D-15                 1.085508427D+04 1.458544515D+01
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S2-                Gurvich,1989 pt1 p274 pt2 p166.
 2 tpis89 S   2.00E   1.00    0.00    0.00    0.00 0   64.1305486     -37132.385
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9597.115
 1.025558251D+04-6.166128250D+02 8.182052840D+00-8.311203580D-03 9.720274160D-06
-5.775476780D-09 1.393690695D-12                -3.063559874D+03-1.906068041D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9597.115
 4.830204030D+05-1.319171302D+03 6.031778480D+00-7.965560690D-04 2.282241690D-07
-2.504364698D-11 7.280550780D-16                 2.660258490D+03-9.010480319D+00
S2CL2              Chase,1998 p859 6/78.
 2 g12/00 S   2.00CL  2.00    0.00    0.00    0.00 0  135.0360000     -16736.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16520.761
 7.974974740D+04-1.636770024D+03 1.583744686D+01-1.186906072D-02 1.413008027D-05
-8.484903930D-09 1.981743887D-12                3.276872420D+03-5.293745205D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16520.761
 6.328816000D+05-3.442705800D+03 1.519637350D+01-2.960877176D-03 6.888284370D-07
-7.990692530D-11 3.692466060D-15                1.526672656D+04-5.453315445D+01
S2F2               Thiothionyl fluoride. Chase,1998 p1147.
 2 j 6/76 S   2.00F   2.00    0.00    0.00    0.00 0  102.1268064     -401413.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13717.892
 1.252904041D+05-1.941243874D+03 1.325382183D+01-1.341525124D-03-2.772465632D-06
 3.658169290D-09-1.299531209D-12               -4.067208250D+04-4.560828617D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13717.892
-2.591757719D+05-1.059653069D+02 1.006588551D+01-2.274618148D-05 5.412343140D-09
-9.911387140D-13 9.621861440D-17                -5.147675180D+04-2.375666140D+01
S2O                Gurvich,1989 pt1 p293 pt2 p178.
 2 tpis89 S   2.00O   1.00    0.00    0.00    0.00 0   80.1294000     -56035.495
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11128.557
 1.092703310D+04-9.523099870D+01 3.144525430D+00 1.176854200D-02-1.580266840D-05
 1.037645040D-08-2.708622260D-12               -7.500471900D+03 1.104169896D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11128.557
-1.442139790D+05-3.276430130D+02 7.244286110D+00-9.776538300D-05 2.162712700D-08
-2.482782220D-12 1.151778750D-16                -7.438553930D+03-1.085180744D+01
S3                 Gurvich,1989 pt1 p275 pt2 p167.
 2 tpis89 S   3.00    0.00    0.00    0.00    0.00 0   96.1950000     144738.328
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11974.328
 7.245395740D+04-1.162146759D+03 9.955413680D+00-4.158026220D-03 3.241778390D-06
-1.264648239D-09 1.777450535D-13                2.146275475D+04-2.587525865D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11974.328
-1.117805401D+05-5.197908390D+01 7.038760840D+00-1.546804022D-05 3.408340410D-09
-3.896862360D-13 1.800860389D-17                1.525406485D+04-7.610045099D+00
S4                 Gurvich,1989 pt1 p280 pt2 p168.
 2 tpis89 S   4.00    0.00    0.00    0.00    0.00 0  128.2600000     135632.333
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14280.333
 1.198664135D+05-2.040786521D+03 1.510235054D+01-7.041104300D-03 5.350405000D-06
-2.002348038D-09 2.569940995D-13                2.410909409D+04-5.503153238D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14280.333
-2.068333537D+05-9.696151430D+01 1.007243210D+01-2.895047053D-05 6.387806190D-09
-7.311767430D-13 3.382265290D-17                1.321109530D+04-2.344872237D+01
S5                 Gurvich,1989 pt1 p281 pt2 p169.
 2 tpis89 S   5.00    0.00    0.00    0.00    0.00 0  160.3250000     132993.354
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19053.354
 1.361370439D+05-2.955476536D+03 2.633358816D+01-4.125806530D-02 7.056814030D-05
-5.611095330D-08 1.659457200D-11                2.675307046D+04-1.069711067D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19053.354
-4.038495160D+06 8.601803880D+03 7.443780900D+00 1.533393812D-03-2.532718676D-07
 2.145210795D-11-7.213102680D-16               -4.686925420D+04 1.104229196D+01
S6                 Gurvich,1989 pt1 p282 pt2 p170.
 2 tpis89 S   6.00    0.00    0.00    0.00    0.00 0  192.3900000     101315.180
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22787.179
 9.780307210D+04-2.568470130D+03 2.467025557D+01-1.619983175D-02 1.712334526D-05
-9.746296740D-09 2.486964867D-12                2.037888389D+04-1.014410309D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22787.179
 3.686845060D+06-7.695017900D+03 1.860721995D+01 2.290382548D-03-1.219834021D-06
 2.060780798D-10-1.190354318D-14                6.032486480D+04-7.490245718D+01
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S7                Gurvich,1989 pt1 p283 pt2 p171.
 2 tpis89 S   7.00     0.00     0.00     0.00     0.00 0  224.4550000      111890.369
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26274.368
 1.233655613D+05-3.200543640D+03 3.015678887D+01-2.197472483D-02 2.487892075D-05
-1.506049557D-08 3.768925990D-12                 2.390005896D+04-1.275978171D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26274.368
-2.726396041D+05-7.373215220D+01 1.905771987D+01-2.394575885D-05 5.442671300D-09
-6.379663480D-13 3.008212993D-17                 7.308458830D+03-6.159112428D+01
S8                Gurvich,1989 pt1 p284 pt2 p172.
 2 tpis89 S   8.00     0.00     0.00     0.00     0.00 0  256.5200000      101277.122
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31573.122
 3.145625719D+05-6.116510160D+03 4.875327540D+01-6.241794650D-02 7.421831750D-05
-3.726449310D-08 5.799429880D-12                 3.573890840D+04-2.288701977D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31573.122
-8.727921130D+06 1.221627968D+04 2.209959617D+01-3.494064830D-03 1.397604162D-06
-2.169815281D-10 1.212304364D-14                -8.658110820D+04-6.435742508D+01
Sc                Hf:Gurvich,1982. Sugar,1985. Gordon,1999.
 3 g 1/99 SC  1.00     0.00     0.00     0.00     0.00 0   44.9559100      377700.259
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7002.259
-3.700805940D+03 1.692506026D+02 1.842242597D+00 1.364835821D-03-1.580085847D-06
 9.613111150D-10-2.392381918D-13                 4.385215240D+04 1.072781921D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7002.259
 8.810382650D+06-2.711232975D+04 3.476588660D+01-1.861104581D-02 5.290283900D-06
-6.585408060D-10 2.997850429D-14                 2.162460097D+05-2.225618519D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7002.259
 2.283130511D+09-1.367701232D+06 3.213593060D+02-3.563171100D-02 2.093254715D-06
-6.238650020D-11 7.425605615D-16                 1.092708359D+07-2.781409383D+03
Sc+               Sugar,1985. Gordon,1999.
 3 g 7/97 SC  1.00E  -1.00     0.00     0.00     0.00 0   44.9553614     1017145.222
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7161.922
-5.884930160D+03 1.479044408D+02 2.009576456D+00 7.389566970D-04-6.617964820D-07
 6.841073760D-10-2.164125532D-13                 1.208439139D+05 1.026570620D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7161.922
 1.973658531D+06-4.954384100D+03 6.360627350D+00-7.168785920D-04 2.464991123D-08
 9.632373790D-12-8.544709642D-16                 1.543423764D+05-2.261925782D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7161.922
 2.219151811D+08-1.287881370D+05 3.265593870D+01-3.379963200D-03 1.981741972D-07
-5.190207160D-12 4.635586113D-17                 1.149364313D+06-2.553294937D+02
Sc-               Hotop,1985. Used J from isoelectronic Ti. Gordon,1999.
 3 g 9/97 SC  1.00E   1.00     0.00     0.00     0.00 0   44.9564586      352558.828
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 4.165746390D+04 8.270420720D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 4.165746390D+04 8.270420720D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 4.165746390D+04 8.270420720D+00
ScO               D0,Props(extrap):Gurvich,1982 pt1 p140 pt2 p143.
 3 tpis89 SC  1.00O   1.00     0.00     0.00     0.00 0   60.9553100      -55065.294
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8787.106
-3.136784613D+03 2.271981685D+02 8.850757320D-01 1.052430774D-02-1.431954596D-05
 9.652351070D-09-2.586210633D-12                -8.550798770D+03 2.012706847D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8787.106
 1.224192443D+06-3.918915720D+03 8.679848810D+00-1.995893306D-03 4.066989850D-07
-1.504459913D-11-8.472998900D-16                 1.677322594D+04-2.951656272D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8787.106
 5.435720930D+08-2.629571561D+05 4.324788690D+01-8.590816240D-04-1.205059380D-07
 6.918221540D-12-1.109417319D-16                 2.162498313D+06-3.650332350D+02
ScO+              D0,Estim.cons:Gurvich,1982 pt1 p142 pt2 p145.
 3 g10/99 SC  1.00O   1.00E  -1.00     0.00     0.00 0   60.9547614      561209.966
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8777.066
 4.588560270D+04-3.367114370D+02 3.527206400D+00 3.988850300D-03-5.568985430D-06
 3.650281190D-09-9.356491500D-13                 6.838350790D+04 4.339812700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8777.066
-1.814357141D+06 5.853425320D+03-3.657101210D+00 5.734364510D-03-2.092878161D-06
 3.695645020D-10-2.214038347D-14                 2.955364078D+04 5.660889410D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8777.066
 4.395803280D+09-2.670232109D+06 6.250769670D+02-6.991767580D-02 4.175372710D-06
-1.274326266D-10 1.571603736D-15                 2.130530393D+07-5.428823800D+03
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ScO2              Gurvich,1982 pt1 p143 pt2 p147.
 2 tpis82 SC  1.00O   2.00    0.00    0.00    0.00 0   76.9547100    -413650.667
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10752.133
 4.794700960D+04-4.298358590D+02 3.417206500D+00 1.361338544D-02-2.047465023D-05
 1.455906041D-08-4.038087690D-12                -4.861049530D+04 7.670013330D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10752.133
-1.903902542D+05-2.315588820D+02 7.172104910D+00-6.859209640D-05 1.510998557D-08
-1.727951588D-12 7.988980500D-17                -5.112974750D+04-1.090764597D+01
Sc2O              Gurvich,1982 pt1 p144 pt2 p148.
 2 tpis82 SC  2.00O   1.00    0.00    0.00    0.00 0  105.9112200     -23044.208
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11709.844
 2.550002615D+04-3.077608607D+02 4.671215040D+00 8.696142250D-03-1.283873116D-05
 8.988966810D-09-2.461994147D-12                -2.614951944D+03 2.920017180D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11709.844
-1.350880396D+05-1.854540692D+02 7.138294080D+00-5.529432140D-05 1.221589315D-08
-1.400490463D-12 6.488858110D-17                -4.240235140D+03-9.372710950D+00
Sc2O2             Gurvich,1982 pt1 p145 pt2 p149.
 2 tpis82 SC  2.00O   2.00    0.00    0.00    0.00 0  121.9106200     -490571.020
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13133.780
 3.468445490D+03 2.617988314D+02-3.052099624D-01 3.076104070D-02-4.183478360D-05
 2.794218425D-08-7.412672050D-12                -6.144013210D+04 2.915248555D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13133.780
-2.977348677D+05-5.803677920D+02 1.043318377D+01-1.734165462D-04 3.836089790D-08
-4.403078030D-12 2.042208922D-16                -5.964866280D+04-2.855828369D+01
Si                Hf:Cox,1989. NIST data version1.1 [Online]1997. Gordon,1999.
 3 g 8/97 SI  1.00    0.00    0.00    0.00    0.00 0   28.0855000     450000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7550.258
 9.836140810D+01 1.546544523D+02 1.876436670D+00 1.320637995D-03-1.529720059D-06
 8.950562770D-10-1.952873490D-13                 5.263510310D+04 9.698288880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7550.258
-6.169298850D+05 2.240683927D+03-4.448619320D-01 1.710056321D-03-4.107714160D-07
 4.558884780D-11-1.889515353D-15                 3.953558760D+04 2.679668061D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7550.258
-9.286548940D+08 5.443989890D+05-1.206739736D+02 1.359662698D-02-7.606498660D-07
 2.149746065D-11-2.474116774D-16                -4.293792120D+06 1.086382839D+03
Si+               Martin,1983. Gordon,1999.
 3 g 4/97 SI  1.00E  -1.00    0.00    0.00    0.00 0   28.0849514    1242508.045
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7342.945
-4.329791880D+04 6.795894490D+02 2.257046144D-01 4.118600490D-03-4.234881600D-06
 2.327995626D-09-5.318388059D-13                 1.452039813D+05 1.934650510D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7342.945
 5.919390230D+04-4.856730950D+01 2.556312024D+00-3.503397160D-05 1.190298787D-08
-2.082923821D-12 1.471452049D-16                 1.491431392D+05 5.244267140D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7342.945
-4.364077210D+07 2.434350601D+04-2.763336522D+00 5.924483200D-04-4.454048310D-08
 2.509351585D-12-5.090212919D-17                -4.683214410D+04 5.196564190D+01
Si-               Chase,1998 p1887 3/83. EA:Hotop,1985. Gordon,1999.
 3 g 4/97 SI  1.00E   1.00    0.00    0.00    0.00 0   28.0860486     308817.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-7.940146670D+02 5.567418420D+00 2.499837183D+00-9.481394460D-05 3.171246930D-07
-4.191323180D-10 2.035924380D-13                 3.636443380D+04 5.270119840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-6.162070100D+06 1.883310402D+04-1.899302450D+01 1.111021657D-02-2.535790208D-06
 2.699962923D-10-1.105062911D-14                -8.314089310D+04 1.595298253D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-5.429517960D+07 3.297105700D+04-2.470579690D+00 3.966577600D-04-1.764141255D-08
 4.115769760D-13-3.904369380D-18                -2.315881505D+05 5.226601830D+01
SiBr              Gurvich,1991 pt1 p280 pt2 p249.
 2 tpis91 SI  1.00BR  1.00    0.00    0.00    0.00 0  107.9895000     175157.421
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10035.121
 7.370283350D+03-5.051062960D+02 8.280591040D+00-1.005383920D-02 1.357050920D-05
-9.115449900D-09 2.447477685D-12                 2.184405475D+04-1.662032657D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10035.121
 1.317799940D+06-3.669795020D+03 8.511686120D+00-1.987602041D-03 5.035414890D-07
-4.490120190D-11 8.235670070D-16                 4.332851550D+04-2.467075472D+01
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SiBr2              Gurvich,1991 pt1 p281 pt2 p250.
 2 tpis91 SI  1.00BR  2.00    0.00    0.00    0.00 0  187.8935000     -51000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13317.161
 2.386616151D+04-6.415693470D+02 9.345879110D+00-4.792904140D-03 5.582538470D-06
-3.455312380D-09 8.800338940D-13                -5.014757020D+03-1.740767596D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13317.161
-5.147343940D+04-1.277719997D+01 7.010202240D+00-4.296331860D-06 9.877651970D-10
-1.168133105D-13 5.546681380D-18                -8.319542250D+03-3.611826610D+00
SiBr3              Gurvich,1991 pt1 p282 pt2 p251.
 2 tpis91 SI  1.00BR  3.00    0.00    0.00    0.00 0  267.7975000     -157000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17461.440
 3.972806860D+04-1.066475023D+03 1.380836232D+01-7.641114720D-03 8.775865830D-06
-5.372430850D-09 1.356453455D-12                -1.651795623D+04-3.784055370D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17461.440
-8.888024740D+04-2.267879074D+01 1.001791167D+01-7.481150750D-06 1.709242690D-09
-2.011596627D-13 9.515534150D-18                -2.203026938D+04-1.537574366D+01
SiBr4              Gurvich,1991 pt1 p283 pt2 p252.
 2 tpis91 SI  1.00BR  4.00    0.00    0.00    0.00 0  347.7015000     -415800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22313.721
 6.821086740D+04-1.520370776D+03 1.810453360D+01-9.734688420D-03 1.072367466D-05
-6.343858290D-09 1.557228200D-12                -4.616585210D+04-5.976120630D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22313.721
-1.271409281D+05-3.768087950D+01 1.302910642D+01-1.194958251D-05 2.693843051D-09
-3.137193207D-13 1.471642663D-17                -5.408998830D+04-2.940384330D+01
SiC                Gurvich,1991 pt1 p301 pt2 p265.
 2 tpis91 SI  1.00C   1.00    0.00    0.00    0.00 0   40.0962000      734946.140
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9217.111
-6.223330890D+03 3.141790457D+02 3.893130830D-01 1.187507540D-02-1.639277197D-05
 1.131808223D-08-3.045324231D-12                 8.606227730D+04 2.310166717D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9217.111
-6.268806030D+04 7.209836920D+02 2.162879732D+00 2.201299585D-03-6.569466590D-07
 9.177110260D-11-4.969166740D-15                 8.321225850D+04 1.601675317D+01
SiC2               Gurvich,1991 pt1 p302 pt2 p266.
 2 tpis91 SI  1.00C   2.00    0.00    0.00    0.00 0   52.1069000      631360.938
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11685.409
-4.119628990D+04 6.869747180D+02 2.361343691D-02 1.532939217D-02-1.435588838D-05
 6.375228740D-09-1.059204957D-12                 7.130890710D+04 2.828850316D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11685.409
 7.026893090D+06-2.466148437D+04 3.915453030D+01-2.002884068D-02 6.307353690D-06
-8.848383510D-10 4.530549850D-14                 2.267325155D+05-2.366622024D+02
SiCL               Gurvich,1991 pt1 p271 pt2 p243.
 2 tpis91 SI  1.00CL  1.00    0.00    0.00    0.00 0   63.5385000      142363.219
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9884.119
 1.248508319D+04-2.044170347D+02 4.977070850D+00-5.160756260D-04 2.931980374D-07
-3.666615230D-12-3.393037130D-14                 1.686528019D+04-2.263957240D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9884.119
 3.767294560D+05-1.147956509D+03 5.735408430D+00-5.784890810D-04 1.517304648D-07
-1.291391394D-11 1.554628420D-16                 2.306278401D+04-6.098515228D+00
SiCL2              Gurvich,1991 pt1 p273 pt2 p244.
 2 tpis91 SI  1.00CL  2.00    0.00    0.00    0.00 0   98.9915000     -163069.287
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12529.294
 5.305550970D+04-1.015842786D+03 1.032848185D+01-6.212267520D-03 6.715825400D-06
-3.908801640D-09 9.461732150D-13                -1.650218093D+04-2.649925756D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12529.294
-8.050871570D+04-2.661025523D+01 7.020414720D+00-8.335824720D-06 1.871092411D-09
-2.171552767D-13 1.015849895D-17                -2.181294885D+04-6.638764238D+00
SiCL3              Gurvich,1991 pt1 p275 pt2 p245.
 2 tpis91 SI  1.00CL  3.00    0.00    0.00    0.00 0  134.4445000     -336271.670
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15717.467
 8.691708460D+04-1.677556857D+03 1.511519060D+01-8.937031000D-03 9.097353530D-06
-5.014579960D-09 1.155962016D-12                -3.477477300D+04-5.087215506D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15717.467
-1.477180114D+05-5.335200980D+01 1.004043521D+01-1.635121060D-05 3.641940110D-09
-4.200600590D-13 1.955201587D-17                -4.360571650D+04-2.006632444D+01
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SiCL4              Gurvich,1991 pt1 p276 pt2 p246.
 2 tpis91 SI  1.00CL  4.00    0.00    0.00    0.00 0  169.8975000    -662200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19455.438
 1.171646285D+05-2.185821461D+03 1.908250496D+01-9.636335720D-03 8.836847690D-06
-4.360042400D-09 8.940232430D-13                -7.212802110D+04-7.301532221D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19455.438
-2.100330761D+05-8.476107710D+01 1.306364027D+01-2.554020420D-05 5.653818470D-09
-6.488752670D-13 3.008025543D-17                -8.372268130D+04-3.592584781D+01
SiF                Gurvich,1991 pt1 p264 pt2 p238.
 2 tpis91 SI  1.00F   1.00    0.00    0.00    0.00 0   47.0839032     -25232.686
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9456.114
 1.478223768D+04 1.357998649D+01 2.324182643D+00 7.132851180D-03-1.022951215D-05
 7.148396470D-09-1.964689785D-12                -3.995380650D+03 1.231128121D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9456.114
-3.653637880D+05 8.722860040D+02 3.377218270D+00 7.508152430D-04-2.308898619D-07
 3.766781800D-11-2.143080403D-15                -1.011697664D+04 8.968132820D+00
SiFCL              Gurvich,1991 pt1 p279 pt2 p248.
 2 tpis91 SI  1.00F   1.00CL  1.00    0.00    0.00 0   82.5369032     -377826.516
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11832.884
 4.176954640D+04-5.926575380D+02 6.409770710D+00 4.641682610D-03-7.978461910D-06
 6.008728370D-09-1.720953157D-12                -4.398296070D+04-6.259737448D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11832.884
-1.284698945D+05-1.247550173D+02 7.092893850D+00-3.707311770D-05 8.175173010D-09
-9.356435210D-13 4.328544340D-17                -4.723309720D+04-8.337392708D+00
SiF2               Gurvich,1991 pt1 p266 pt2 p239.
 2 tpis91 SI  1.00F   2.00    0.00    0.00    0.00 0   66.0823064     -592838.108
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11204.470
 4.053236650D+04-3.997637560D+02 4.055303880D+00 1.153423049D-02-1.757586754D-05
 1.260369111D-08-3.517105220D-12                -7.047770460D+04 3.879854420D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11204.470
-1.675200202D+05-1.846212090D+02 7.136986350D+00-5.450769860D-05 1.199012961D-08
-1.369470187D-12 6.324889990D-17                -7.287401020D+04-1.117933348D+01
SiF3               Gurvich,1991 pt1 p268 pt2 p240
 2 tpis91 SI  1.00F   3.00    0.00    0.00    0.00 0   85.0807096     -996436.577
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13018.554
 5.755369980D+04-7.179595770D+02 5.379396940D+00 1.813065142D-02-2.738373356D-05
 1.946519470D-08-5.390790560D-12                -1.177631169D+05-3.442902040D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13018.554
-2.903283702D+05-3.427876940D+02 1.025536335D+01-1.019796690D-04 2.250326132D-08
-2.577117181D-12 1.192923177D-16                -1.218088967D+05-2.725261142D+01
SiF4               Johnson,1986. McDowell,1982. Chase,1998 p1190 (6/76).
 2 g 6/01 SI  1.00F   4.00    0.00    0.00    0.00 0  104.0791128    -1615780.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15365.713
 1.069670784D+04-9.569638640D+01 2.513988593D+00 3.309781030D-02-4.573044080D-05
 3.091834452D-08-8.269304050D-12                -1.956252529D+05 1.133722022D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15365.713
-3.845892320D+05-6.569979910D+02 1.348925720D+01-5.100471360D-05 5.346329580D-08
-4.959598110D-12 2.299314375D-16                -1.957284479D+05-4.673894650D+01
SiH                Gurvich,1991 pt1 p257 pt2 p234.
 2 tpis91 SI  1.00H   1.00    0.00    0.00    0.00 0   29.0934400     368636.210
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9145.110
-6.426676300D+03 7.417251210D+01 3.973491600D+00-4.149408880D-03 1.022918384D-05
-8.592386360D-09 2.567093743D-12                4.281745800D+04 2.246937150D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9145.110
 4.042086490D+05-2.364796524D+03 7.627499140D+00-2.496591233D-03 1.108436410D-06
-1.943991955D-10 1.136251507D-14                5.704737680D+04-2.448054429D+01
SiH+               Chase,1998 p1308.
 2 j12/71 SI  1.00H   1.00E  -1.00    0.00    0.00 0   29.0928914    1147671.167
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8654.261
-4.307157170D+04 3.884958240D+02 2.546166863D+00-6.686325980D-04 5.186277020D-06
-4.818569740D-09 1.445702640D-12                1.349079707D+05 9.027950090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8654.261
 1.711692033D+05-1.045807287D+03 4.838648240D+00 1.277940891D-04-6.883872450D-08
 1.418843480D-11-7.855316960D-16                1.431721450D+05-7.553299140D+00
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SiHBr3            Chase,1998 p514.
 2 j12/76 SI  1.00H   1.00BR  3.00    0.00    0.00 0  268.8054400    -302922.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17823.429
 1.322811122D+05-2.205365507D+03 1.775084194D+01-1.047794569D-02 1.286821723D-05
-7.743124260D-09 1.819060891D-12                -2.834992682D+04-6.331199540D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17823.429
 2.199973526D+05-2.024458552D+03 1.435781007D+01-5.037015840D-04 1.054049755D-07
-1.160828765D-11 5.217257680D-16                -2.842086214D+04-4.536437170D+01
SiHCL             Gurvich,1991 pt1 p277 pt2 p247.
 2 tpis91 SI  1.00H   1.00CL  1.00    0.00    0.00 0   64.5464400      54945.913
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10665.413
 5.909673050D+04-8.780064030D+02 7.999687930D+00-4.663141270D-03 8.594986000D-06
-6.608073550D-09 1.868076396D-12                 9.567570340D+03-1.690014311D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10665.413
 1.012152890D+05-1.163239598D+03 7.376366550D+00 1.874151313D-04-1.661351093D-07
 3.964414040D-11-2.640580080D-15                 1.141064087D+04-1.507678798D+01
SiHCL3            Chase,1998 880.
 2 j12/76 SI  1.00H   1.00CL  3.00    0.00    0.00 0  135.4524400    -496222.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16151.608
 1.659565586D+05-2.552498122D+03 1.750117375D+01-7.885728660D-03 8.092567490D-06
-3.980420600D-09 7.059173320D-13                -4.951316600D+04-6.758519053D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16151.608
 1.728644072D+05-2.116727327D+03 1.441802307D+01-5.255249620D-04 1.098826178D-07
-1.209327059D-11 5.432187050D-16                -5.130351940D+04-5.036360893D+01
SiHF              Gurvich,1991 pt1 p270 pt2 p242.
 2 tpis91 SI  1.00H   1.00F   1.00    0.00    0.00 0   48.0918432    -162657.169
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10230.231
 2.192598671D+04-6.175229080D+01 2.127372739D+00 1.123538312D-02-1.322503985D-05
 8.307307390D-09-2.010545971D-12                -2.016994845D+04 1.367184876D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10230.231
 4.049752240D+06-9.295526820D+03 1.071754366D+01 1.868124220D-03-1.129820372D-06
 1.960250100D-10-1.144682011D-14                 4.133225200D+04-4.736317600D+01
SiHF3             Chase,1998 p1160.
 2 j 6/76 SI  1.00H   1.00F   3.00    0.00    0.00 0   86.0886496   -1200808.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13544.634
 8.325879390D+04-8.178594460D+02 4.041717240D+00 2.726104628D-02-3.787831480D-05
 2.630589305D-08-7.289582500D-12                -1.416146961D+05 1.382806532D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13544.634
 7.820100800D+04-2.592742261D+03 1.475104214D+01-6.531047200D-04 1.372428937D-07
-1.516371051D-11 6.832497150D-16                -1.336611887D+05-5.851450950D+01
SiHI3             Chase,1998 p1266.
 2 j12/76 SI  1.00H   1.00I   3.00    0.00    0.00 0  409.8068500     -74475.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19135.424
 1.113840054D+05-1.974457175D+03 1.791396249D+01-1.219208519D-02 1.613169233D-05
-1.038096942D-08 2.613287761D-12                -2.256377425D+03-5.995455130D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19135.424
 2.279424252D+05-1.898603142D+03 1.428134804D+01-4.776026950D-04 1.003097496D-07
-1.107859145D-11 4.990338200D-16                -1.614547674D+03-4.122943070D+01
SiH2              Gurvich,1991 pt1 p260. Fredin,1985. Dubois,1968.
 2 g 3/01 SI  1.00H   2.00    0.00    0.00    0.00 0   30.1013800     273332.530
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10018.102
-2.063863564D+04 3.305862200D+02 2.099271145D+00 3.542539370D-03 3.378876670D-06
-5.383845620D-09 2.081191273D-12                 3.011784298D+04 1.282333570D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10018.102
 4.624039370D+06-1.143436110D+04 1.264880870D+01 9.114899500D-04-8.766611540D-07
 1.646297357D-10-9.965090370D-15                 1.072475101D+05-6.606078070D+01
SiH2Br2           Chase,1998 p481.
 2 j12/76 SI  1.00H   2.00BR  2.00    0.00    0.00 0  189.9093800    -190372.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14272.222
 1.651528003D+05-2.468145554D+03 1.608639427D+01-9.413840900D-03 1.407423872D-05
-9.240751450D-09 2.255641666D-12                -1.276482614D+04-5.945374320D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14272.222
 5.665851440D+05-3.973919620D+03 1.567387912D+01-9.943802290D-04 2.084856022D-07
-2.299521351D-11 1.034736283D-15                -2.990690180D+03-6.190476520D+01
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SiH2CL2           Chase,1998 p823.
 2 j12/76 SI  1.00H   2.00CL  2.00    0.00    0.00 0  101.0073800    -320494.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13384.948
 1.894281754D+05-2.650960252D+03 1.549874174D+01-6.533130750D-03 9.306098260D-06
-5.639698670D-09 1.213664264D-12               -2.720912007D+04-6.006331649D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13384.948
 5.400204580D+05-4.062337290D+03 1.573118788D+01-1.015038389D-03 2.127060243D-07
-2.345079226D-11 1.054871984D-15               -1.823098225D+04-6.544540499D+01
SiH2F2            Chase,1998 p1108.
 2 j 6/76 SI  1.00H   2.00F   2.00    0.00    0.00 0   68.0981864    -790776.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11988.206
 1.272188427D+05-1.241724310D+03 4.899435890D+00 2.123882008D-02-2.725708700D-05
 1.860857446D-08-5.226604330D-12               -8.980466920D+04-5.111815500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11988.206
 4.726534080D+05-4.388517690D+03 1.596032597D+01-1.102993658D-03 2.315838331D-07
-2.556974559D-11 1.151499711D-15               -7.316184460D+04-7.098989270D+01
SiH2I2            Chase,1998 p1313.
 2 j12/76 SI  1.00H   2.00I   2.00    0.00    0.00 0  283.9103200     -38074.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14917.266
 1.539963319D+05-2.414436989D+03 1.684409354D+01-1.212037580D-02 1.808453226D-05
-1.207740133D-08 3.040799276D-12               5.073073250D+03-6.098720820D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14917.266
 5.942390830D+05-3.924814480D+03 1.563850289D+01-9.805706340D-04 2.054871384D-07
-2.265587199D-11 1.019168663D-15               1.513627352D+04-5.940812520D+01
SiH3              Gurvich,1991 pt1 p261 pt2 p236.
 2 g 3/99 SI  1.00H   3.00    0.00    0.00    0.00 0   31.1093200     204357.366
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10276.989
 4.341142820D+03 2.277185085D+02 6.508250350D-01 1.221438558D-02-4.347604270D-06
-1.774916828D-09 1.184191367D-12               2.259993826D+04 1.968347482D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10276.989
 6.056321220D+05-4.721254060D+03 1.329129523D+01-1.256824868D-03 2.688285940D-07
-3.010741582D-11 1.370945857D-15               4.974420640D+04-6.140503100D+01
SiH3Br            Chase,1998 p439.
 2 j12/76 SI  1.00H   3.00BR  1.00    0.00    0.00 0  111.0133200     -78241.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11769.378
 1.521065525D+05-1.987744479D+03 1.131460743D+01-1.806099407D-03 7.769262470D-06
-6.233478170D-09 1.585331846D-12              -9.248868880D+02-3.846463690D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11769.378
 9.279285780D+05-5.917935790D+03 1.699209298D+01-1.487507364D-03 3.123451161D-07
-3.449071470D-11 1.553431675D-15               2.241560128D+04-7.948611590D+01
SiH3CL            Chase,1998 p764.
 2 j12/76 SI  1.00H   3.00CL  1.00    0.00    0.00 0   66.5623200    -141838.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11440.706
 1.633388301D+05-2.030302118D+03 1.068016138D+01 4.942370140D-04 4.305174760D-06
-3.748327270D-09 8.893504210D-13              -8.180714980D+03-3.688956824D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11440.706
 9.087780940D+05-5.958949560D+03 1.702076016D+01-1.498450667D-03 3.146813781D-07
-3.475168460D-11 1.565281681D-15               1.493793206D+04-8.127277864D+01
SiH3F             Chase,1998 p1058.
 2 j 6/76 SI  1.00H   3.00F   1.00    0.00    0.00 0   50.1077232    -376560.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10931.622
 1.267836290D+05-1.177593516D+03 4.499188960D+00 1.658543011D-02-1.678598921D-05
 1.019153931D-08-2.803920232D-12              -4.010392970D+04-4.481080920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10931.622
 8.624313170D+05-6.103370570D+03 1.712733597D+01-1.540724131D-03 3.239628720D-07
-3.581056890D-11 1.614151380D-15              -1.261487616D+04-8.399227210D+01
SiH3I             Chase,1998 p1342.
 2 j12/76 SI  1.00H   3.00I   1.00    0.00    0.00 0  158.0137900     -2092.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12078.229
 1.459384799D+05-1.982982746D+03 1.196516737D+01-3.937505950D-03 1.087991733D-05
-8.433135920D-09 2.196078188D-12               8.063208310D+03-4.064553320D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12078.229
 9.361149180D+05-5.859720290D+03 1.695376698D+01-1.473497130D-03 3.094475885D-07
-3.417462470D-11 1.539334807D-15               3.127499231D+04-7.801700080D+01
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SiH4              Silane. Gurvich,1991 pt1 p263 pt 2 p237.
 2 tpis91 SI  1.00H   4.00     0.00     0.00     0.00 0   32.1172600       34700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10535.001
 7.872993290D+04-5.526087050D+02 2.498944303D+00 1.442118274D-02-8.467107310D-06
 2.726164641D-09-5.436754370D-13                 6.269669060D+03 4.965461830D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10535.001
 1.290378740D+06-7.813399780D+03 1.828851664D+01-1.975620946D-03 4.156502150D-07
-4.596745610D-11 2.072777131D-15                 4.766887950D+04-9.801697460D+01
SiI               Gurvich,1991 pt1 p284 pt2 p253.
 2 tpis91 SI  1.00I   1.00     0.00     0.00     0.00 0  154.9899700      262953.420
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9941.120
 9.492081340D+04-1.573960062D+03 1.237908109D+01-1.593864820D-02 1.692049005D-05
-9.215558320D-09 2.046186848D-12                 3.779735670D+04-4.066407850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9941.120
 8.529402790D+05-2.442039471D+03 7.722977520D+00-1.985601243D-03 6.542866630D-07
-9.494158290D-11 4.890041370D-15                 4.578160940D+04-1.733975081D+01
SiI2              Chase,1998 p1432.
 2 j12/76 SI  1.00I   2.00     0.00     0.00     0.00 0  281.8944400       92466.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13792.515
 1.163352403D+04-4.514482170D+02 8.707978130D+00-3.580664930D-03 4.253714430D-06
-2.673478266D-09 6.891558980D-13                 1.126247142D+04-1.155818335D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13792.515
 1.002168907D+04 1.433017148D+01 6.701330550D+00 3.960769900D-04-2.073866165D-07
 4.553457100D-11-3.016798280D-15                 9.007368100D+03 2.887336913D-01
SiN               Gurvich,1991 pt1 p295 pt2 p261.
 2 g 5/99 SI  1.00N   1.00     0.00     0.00     0.00 0   42.0922000      403668.437
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8736.137
-1.464672152D+04 1.374993497D+02 3.678508580D+00-6.158499200D-03 2.309417067D-05
-2.294461481D-08 7.395665680D-12                 4.673212990D+04 6.494564115D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8736.137
-2.932685132D+06 5.853688590D+03 1.321451677D+00 1.258329284D-03-3.773886360D-07
 6.887761040D-11-4.189842590D-15                 6.527148810D+03 2.553145732D+01
SiO               Gurvich,1991 pt1 p247 pt2 p227
 2 tpis91 SI  1.00O   1.00     0.00     0.00     0.00 0   44.0849000      -98842.418
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8715.105
-4.722771050D+04 8.063137640D+02-1.636976133D+00 1.454275546D-02-1.723202046D-05
 1.042397340D-08-2.559365273D-12                -1.666585903D+04 3.355795700D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8715.105
-1.765134162D+05-3.199177090D+01 4.477441930D+00 4.591764710D-06 3.558143150D-08
-1.327012559D-11 1.613253297D-15                -1.350842360D+04-8.386957330D-01
SiO2              Gurvich,1991 pt1 p256 pt2 p233.
 2 tpis91 SI  1.00O   2.00     0.00     0.00     0.00 0   60.0843000     -322073.477
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10542.523
-3.362948780D+04 4.734078920D+02 2.309770671D-01 1.850230806D-02-2.242786671D-05
 1.364981554D-08-3.351935030D-12                -4.226487490D+04 2.295803206D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           10542.523
-1.464031193D+05-6.261441060D+02 7.964563710D+00-1.854119096D-04 4.095214670D-08
-4.697206760D-12 2.178054280D-16                -3.791834770D+04-2.045285414D+01
SiS               Gurvich,1991 pt1 p290 pt2 p258.
 2 tpis91 SI  1.00S   1.00     0.00     0.00     0.00 0   60.1505000      108194.407
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8932.107
 3.599449290D+04-4.239723300D+02 4.654014420D+00 1.588470782D-03-3.310254360D-06
 2.706096479D-09-8.113517820D-13                 1.411515571D+04-1.183201858D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8932.107
-2.102323897D+06 6.228836180D+03-3.004120882D+00 4.495499930D-03-1.368821364D-06
 1.998097253D-10-9.882035800D-15                -2.795538166D+04 5.405828786D+01
SiS2              Gurvich,1991 pt1 p294 pt2 p260.
 2 tpis91 SI  1.00S   2.00     0.00     0.00     0.00 0   92.2155000       7022.717
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           12203.217
 4.397745660D+04-7.430013120D+02 7.941588360D+00 2.038083730D-03-4.646337600D-06
 3.848014360D-09-1.157260149D-12                 2.801077853D+03-1.736888325D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           12203.217
-1.266489071D+05-9.774235220D+01 7.572803680D+00-2.905413928D-05 6.405587840D-09
-7.329273340D-13 3.389819780D-17                -1.244672263D+03-1.352710463D+01
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Si2                Gurvich,1991 pt1 p240 pt2 p225.
 2 tpis91 SI  2.00     0.00     0.00     0.00     0.00 0   56.1710000      580195.524
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10296.124
 1.237596221D+04-1.024904376D+02 4.354848520D+00 1.281063335D-03-2.531991623D-06
 2.265694244D-09-7.001290140D-13                 6.906942850D+04 3.251125200D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10296.124
 1.370060657D+06-4.207060040D+03 9.337432890D+00-2.749217168D-03 9.586345960D-07
-1.372449748D-10 6.765028100D-15                 9.510884540D+04-3.168385190D+01
Si2C               Gurvich,1991 pt1 p304 pt2 p267.
 2 tpis91 SI  2.00C    1.00     0.00     0.00     0.00 0   68.1817000      554093.904
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11582.346
-4.553366200D+03 1.314796415D+02 2.469106923D+00 1.276520680D-02-1.656910776D-05
 1.065289663D-08-2.739192976D-12                 6.470049920D+04 1.468838980D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11582.346
-1.253829442D+05-3.414277790D+02 7.254365330D+00-1.017635503D-04 2.250902158D-08
-2.584074852D-12 1.198884876D-16                 6.608009380D+04-1.146216579D+01
Si2F6              Lyman,2001.
 2 g 6/01 SI  2.00F    6.00     0.00     0.00     0.00 0  170.1614192    -2383290.080
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26694.292
 1.580767450D+04-2.975292881D+02 7.512591500D+00 4.552796230D-02-6.421876840D-05
 4.357408730D-08-1.166762282D-11                -2.886707444D+05-7.721784770D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26694.292
-9.186303140D+05 1.573948683D+02 2.141256129D+01-2.681898667D-04 7.212280110D-08
-9.184252660D-12 4.537238360D-16                -2.966176753D+05-7.849022470D+01
Si2N               Chase,1998 p1611.
 2 j 3/67 SI  2.00N    1.00     0.00     0.00     0.00 0   70.1777000      397480.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11822.188
 2.318271938D+04-3.674843790D+02 5.409658600D+00 8.176389400D-03-1.220312934D-05
 8.580609100D-09-2.354927059D-12                 4.809278030D+04-3.042205654D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11822.188
-2.805026986D+05 2.502366876D+02 7.092456100D+00 2.853120795D-04-9.792101810D-08
 1.552154244D-11-8.036260450D-16                 4.342014790D+04-1.009570910D+01
Si3                Gurvich,1991 pt1 p246 pt2 p226.
 2 g 7/95 SI  3.00     0.00     0.00     0.00     0.00 0   84.2565000      627867.381
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12519.793
-1.114208177D+04 1.575785843D+02 2.486135003D+00 1.631637255D-02-2.208240021D-05
 1.372008287D-08-3.262330700D-12                 7.328253850D+04 1.588081347D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12519.793
-1.699395561D+06 4.697815380D+03 2.618198124D+00 1.959082075D-03-2.581160603D-07
 6.103444860D-12 6.086309240D-16                 4.277916810D+04 2.586540384D+01
Sn                 Hf:Cox,1989 Moore,1971. Gordon,1999.
 3 g 7/97 SN  1.00     0.00     0.00     0.00     0.00 0  118.7100000      301200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6214.713
-1.248692263D+05 1.618841190D+03-4.602397350D+00 1.045433308D-02 2.998265550D-06
-1.068699386D-08 4.323421310D-12                 2.748364008D+04 4.805067230D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6214.713
-5.145695640D+06 1.140575108D+04-4.179632060D+00 2.236390679D-03-3.603219770D-07
 2.440237836D-11-2.937628285D-16                -4.215013570D+04 5.981450930D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6214.713
-1.119787114D+09 6.427046040D+05-1.378615913D+02 1.453867222D-02-7.109586030D-07
 1.501409263D-11-8.940758657D-17                -5.111296870D+06 1.245625545D+03
Sn+                Moore,1971. Gordon,1999.
 3 g 7/97 SN  1.00E   -1.00     0.00     0.00     0.00 0  118.7094514     1015949.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
-5.571297780D+03 1.222323189D+02 1.566361415D+00 3.397061410D-03-6.312922290D-06
 5.585452080D-09-1.689021340D-12                 1.209024120D+05 1.162634765D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 4.622916850D+06-1.185958712D+04 1.237026473D+01-2.773624217D-03 3.098513490D-07
-5.362951440D-12-8.663474691D-16                 1.994322977D+05-6.837108280D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 1.913728057D+08-1.145730242D+05 3.070294184D+01-3.387878800D-03 1.966377351D-07
-4.388396290D-12 2.057062343D-17                 1.031631149D+06-2.370157923D+02
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Sn-                Hotop,1985. Gordon,1999.
 3 g 9/97 SN  1.00E   1.00     0.00     0.00     0.00 0  118.7105486      179495.949
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6490.449
 2.722796000D+05-3.369935800D+03 1.743906405D+01-2.810527618D-02 2.790684767D-05
-1.442400675D-08 3.070159757D-12                 3.753227750D+04-8.007856970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6490.449
-6.447713220D+04 7.430555100D+02 1.921380256D+00 2.361623997D-04-5.280668360D-08
 6.102339380D-12-2.843422486D-16                 1.645739414D+04 1.265436865D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6490.449
-1.314284778D+06 8.972354270D+02 2.302354538D+00 2.246840970D-05-1.392571963D-09
 4.468904450D-14-5.811846560D-19                 1.428800599D+04 1.004933765D+01
SnBr               Gurvich,1991 pt1 p378 pt2 p321.
 2 tpis91 SN  1.00BR  1.00     0.00     0.00     0.00 0  198.6140000      75644.020
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9986.120
 2.564193542D+04-5.259122330D+02 7.687410690D+00-9.654205420D-03 1.482863248D-05
-9.942236980D-09 2.475051091D-12                 1.020483889D+04-1.126550396D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9986.120
 1.815578541D+06-6.728264580D+03 1.332464516D+01-4.608102300D-03 1.236439537D-06
-1.528863587D-10 6.971513500D-15                 4.925583090D+04-5.640962780D+01
SnBr2              Gurvich,1991 pt1 p380 pt2 p323.
 2 tpis91 SN  1.00BR  2.00     0.00     0.00     0.00 0  278.5180000     -118974.592
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14595.408
-4.995753060D+03-1.366498896D+02 7.543563850D+00-1.181772507D-03 1.442445852D-06
-9.254217260D-10 2.423731634D-13                -1.575506969D+04-3.595584020D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14595.408
-1.940894091D+04-2.335607932D+00 7.001969260D+00-8.622241870D-07 2.039869794D-10
-2.464780359D-14 1.189850894D-18                -1.644828122D+04-4.349354750D-01
SnBr3              Gurvich,1991 pt1 p381 pt2 p324.
 2 tpis91 SN  1.00BR  3.00     0.00     0.00     0.00 0  358.4220000     -158716.446
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19280.454
-8.050416470D+03-2.897962523D+02 1.114443355D+01-2.475383807D-03 3.010051350D-06
-1.925695320D-09 5.032605090D-13                -2.070066649D+04-1.895965383D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19280.454
-3.893004530D+04-4.990844170D+00 1.000418437D+01-1.824996910D-06 4.305646660D-10
-5.191887930D-14 2.502455595D-18                -2.217299473D+04-1.229854098D+01
SnBr4              Gurvich,1991 pt1 p384 pt2 p326.
 2 tpis91 SN  1.00BR  4.00     0.00     0.00     0.00 0  438.3260000     -324216.982
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25043.018
-5.832840920D+03-4.270198470D+02 1.467466525D+01-3.604263230D-03 4.366686290D-06
-2.785875130D-09 7.265087870D-13                -4.082916450D+04-3.447104360D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25043.018
-5.176812920D+04-7.426126950D+00 1.300619502D+01-2.692587978D-06 6.336759800D-10
-7.627087190D-14 3.671112000D-18                -4.300166340D+04-2.471455118D+01
SnCL               Gurvich,1991 pt1 p370 pt2 p315.
 2 tpis91 SN  1.00CL  1.00     0.00     0.00     0.00 0  154.1630000      34658.816
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9644.116
 3.351549730D+04-6.832208620D+02 8.393917730D+00-1.164434373D-02 1.812159499D-05
-1.261999170D-08 3.295213470D-12                 6.051790890D+03-1.667834578D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9644.116
 7.741605680D+05-3.602048480D+03 9.749059820D+00-2.596198909D-03 6.367712160D-07
-6.754295570D-11 2.484167602D-15                 2.442447662D+04-3.225454098D+01
SnCL2              Gurvich,1991 pt1 p373 pt2 p317.
 2 tpis91 SN  1.00CL  2.00     0.00     0.00     0.00 0  189.6160000     -202648.283
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13681.717
 9.524665900D+03-4.329845640D+02 8.644720280D+00-3.458409610D-03 4.117852030D-06
-2.592639269D-09 6.692363600D-13                -2.432921127D+04-1.299143851D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13681.717
-3.903588490D+04-7.947962680D+00 7.006487620D+00-2.776594714D-06 6.461341420D-10
-7.119067400D-15 3.688131180D-18                -2.654529653D+04-3.368081174D+00
SnCL3              Gurvich,1991 pt1 p374 pt2 p318.
 2 tpis91 SN  1.00CL  3.00     0.00     0.00     0.00 0  225.0690000     -292372.455
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17554.045
 1.760076813D+04-8.142805480D+02 1.306326984D+01-6.395596190D-03 7.574624570D-06
-4.749711460D-09 1.222182656D-12                -3.413430960D+04-3.457679670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17554.045
-7.482966400D+04-1.528523914D+01 1.001240305D+01-5.285581240D-06 1.226095111D-09
-1.459895108D-13 6.968879780D-18                -3.830878270D+04-1.663063137D+01
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SnCL4              Gurvich,1991 pt1 p376 pt2 p320.
 2 tpis91 SN  1.00CL  4.00     0.00     0.00     0.00 0  260.5220000     -478465.969
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22474.031
 4.245967870D+04-1.280574318D+03 1.768445328D+01-9.574779520D-03 1.115620323D-05
-6.907229270D-09 1.759652856D-12                 -5.504009040D+04-5.827352999D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22474.031
-1.078336862D+05-2.554305872D+01 1.302040391D+01-8.595125900D-06 1.976570888D-09
-2.337929994D-13 1.110287624D-17                 -6.163562030D+04-3.072702622D+01
SnF                Gurvich,1991 pt1 p365 pt2 p310.
 2 tpis91 SN  1.00F   1.00     0.00     0.00     0.00 0  137.7084032      -95017.090
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9136.110
 6.098503520D+04-9.860306290D+02 8.994731210D+00-1.223012156D-02 1.840583578D-05
-1.267926607D-08 3.291331020D-12                 -7.882614480D+03-2.221921734D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9136.110
 2.589715476D+04-1.484478214D+03 7.378518930D+00-1.324244440D-03 2.847634043D-07
-2.360371345D-11 6.116783710D-16                 -4.776688970D+03-1.681202516D+01
SnF2               Gurvich,1991 pt1 p368 pt2 p312.
 2 tpis91 SN  1.00F   2.00     0.00     0.00     0.00 0  156.7068064     -510956.951
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12243.049
 7.042391850D+04-1.137505955D+03 1.008659352D+01-4.722855930D-03 4.135702920D-06
-1.921143972D-09 3.640760280D-13                 -5.756670820D+04-2.571566624D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12243.049
-1.027758772D+05-4.451751620D+01 7.033268760D+00-1.329882797D-05 2.934271938D-09
-3.358415920D-13 1.553358669D-17                 -6.362125880D+04-6.810084520D+00
SnF3               Gurvich,1991 pt1 p369 pt2 p313.
 2 tpis91 SN  1.00F   3.00     0.00     0.00     0.00 0  175.7052096     -646630.479
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14799.721
 1.095555529D+05-1.950557979D+03 1.541407832D+01-8.546518770D-03 7.800551820D-06
-3.825942220D-09 7.787747760D-13                 -7.056794920D+04-5.494639480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14799.721
-1.829319689D+05-7.557358680D+01 1.005671455D+01-2.275132668D-05 5.034695820D-09
-5.776530960D-13 2.677214170D-17                 -8.091897590D+04-2.191673972D+01
SnF4               Gurvich,1991 pt1 p369 pt2 p314.
 2 tpis91 SN  1.00F   4.00     0.00     0.00     0.00 0  194.7036128    -1024766.717
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18801.983
 1.390441119D+05-2.168784371D+03 1.691802917D+01-2.318608529D-03-2.045847976D-06
 3.430087900D-09-1.289228860D-12                 -1.153563396D+05-6.370604750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18801.983
-2.635692764D+05-1.445469969D+02 1.310690681D+01-4.237755790D-05 9.286871950D-09
-1.057062694D-12 4.867108680D-17                 -1.271539967D+05-3.803921900D+01
SnI                Gurvich,1991 pt1 p384 pt2 p327.
 2 tpis91 SN  1.00I   1.00     0.00     0.00     0.00 0  245.6144700     172725.022
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10177.122
 2.670212235D+04-5.006026350D+02 7.490673150D+00-8.746346550D-03 1.289688397D-05
-8.211344930D-09 1.936120475D-12                 2.177249172D+04-9.354806850D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10177.122
-5.554991850D+04-1.530457453D+03 7.932601390D+00-2.108885464D-03 7.809803600D-07
-1.348104887D-10 8.207184700D-15                 2.744864953D+04-1.626822892D+01
SnI2               Gurvich,1991 pt1 p387 pt2 p329.
 2 tpis91 SN  1.00I   2.00     0.00     0.00     0.00 0  372.5189400      -8066.737
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14883.263
-5.739254890D+03-9.435024450D+01 7.377956660D+00-8.258348940D-04 1.011687040D-06
-6.508451600D-10 1.708186600D-13                 -2.622644500D+03-9.605814960D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14883.263
-1.559453390D+04-1.594789414D+00 7.001351160D+00-5.935324240D-07 1.407432564D-10
-1.703457321D-14 8.233611710D-19                 -3.100608319D+03 1.235038509D+00
SnI3               Gurvich,1991 pt1 p388 pt2 p330.
 2 tpis91 SN  1.00I   3.00     0.00     0.00     0.00 0  499.4234100      -8017.540
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20309.360
-1.069978099D+04-1.387693540D+02 1.055637633D+01-1.216435658D-03 1.490873499D-06
-9.594499630D-10 2.518810438D-13                 -3.314229880D+03-1.249558209D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20309.360
-2.517534870D+04-2.348282890D+00 1.000199130D+01-8.752764840D-07 2.076464980D-10
-2.514060336D-14 1.215482266D-18                 -4.017055610D+03-9.263908460D+00
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SnI4              Gurvich,1991 pt1 p391 pt2 p332.
 2 tpis91 SN  1.00I   4.00    0.00    0.00    0.00 0  626.3278800     -118854.043
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26745.957
-1.283146793D+04-1.459885093D+02 1.358634885D+01-1.283554646D-03 1.574557147D-06
-1.013990168D-09 2.663370430D-13                 -1.751178045D+04-2.367973168D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          26745.957
-2.801840706D+04-2.474699366D+00 1.300210215D+01-9.250962340D-07 2.196515817D-10
-2.661071614D-14 1.287167546D-18                 -1.825083832D+04-2.027484281D+01
SnO               Gurvich,1991 pt1 p359 pt2 p307.
 2 tpis91 SN  1.00O   1.00    0.00    0.00    0.00 0  134.7094000      21911.054
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8874.107
 2.547788022D+04-2.293583066D+02 3.421593530D+00 4.713300040D-03-7.365971320D-06
 5.379738870D-09-1.519277855D-12                 2.853047679D+03 6.673965270D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8874.107
-2.555955548D+06 7.870053500D+03-5.439768730D+00 6.307819180D-03-2.068871370D-06
 3.307074880D-10-1.848169716D-14                 -4.841663910D+04 7.175952460D+01
SnO2              Gurvich,1991 pt1 p364 pt2 p309.
 2 tpis91 SN  1.00O   2.00    0.00    0.00    0.00 0  150.7088000      11680.180
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11795.680
 4.707674080D+04-6.114568670D+02 6.117433910D+00 7.514014660D-03-1.238371787D-05
 9.220915990D-09-2.632417597D-12                 2.981068066D+03-8.144926410D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11795.680
-1.573558926D+05-1.427316788D+02 7.605700760D+00-4.198008530D-05 9.218742430D-09
-1.051372983D-12 4.849579270D-17                 -5.234531870D+02-1.428360169D+01
SnS               Gurvich,1991 pt1 p394 pt2 p334.
 2 tpis91 SN  1.00S   1.00    0.00    0.00    0.00 0  150.7750000     111099.012
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9301.112
 2.724877813D+04-4.924126380D+02 6.221654730D+00-3.409406960D-03 3.984913680D-06
-2.470702874D-09 6.339341460D-13                 1.452495307D+04-6.791285229D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9301.112
-1.797985129D+06 6.141736320D+03-4.019504880D+00 5.993829180D-03-2.188735204D-06
 3.899542000D-10-2.406563630D-14                 -2.611349815D+04 6.256820705D+01
SnS2              Gurvich,1991 pt1 p397 pt2 p336.
 2 tpis91 SN  1.00S   2.00    0.00    0.00    0.00 0  182.8400000     149645.595
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13635.095
 3.877145410D+04-8.486953940D+02 1.042083990D+01-5.686902670D-03 6.373829770D-06
-3.825158100D-09 9.502480960D-13                 2.006027952D+04-2.723724769D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13635.095
-6.764084050D+04-1.970189679D+01 7.515333870D+00-6.332559180D-06 1.434207625D-09
-1.676383081D-13 7.886911900D-18                 1.565053629D+04-9.922744838D+00
Sn2               Gurvich,1991 pt1 p354 pt2 p305.
 2 tpis91 SN  2.00    0.00    0.00    0.00    0.00 0  237.4200000     421343.737
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11373.137
-1.329666654D+05 1.639179787D+03-1.902868972D+00 1.290431677D-02-1.120542242D-05
 4.502993860D-09-6.056237770D-13                 4.097452710D+04 4.435408030D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11373.137
-4.275783040D+06 1.236421656D+04-8.438336170D+00 7.088056290D-03-1.712012737D-06
 1.805262952D-10-7.058656810D-15                 -3.001418720D+04 1.005138538D+02
Sr                Hf:Gurvich,1996a. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 1/98 SR  1.00    0.00    0.00    0.00    0.00 0   87.6200000     160500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 4.190649840D+00-6.304437580D-02 2.500373027D+00-1.115455943D-06 1.785248643D-09
-1.456209589D-12 4.750132981D-16                 1.855852648D+04 5.555772840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 1.489414410D+07-4.375335050D+04 5.137266280D+01-2.592566025D-02 6.582990000D-06
-6.949611800D-10 2.417779662D-14                 2.977545522D+05-3.454890770D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 5.562233720D+08-6.093193220D+05 2.109096848D+02-3.010063957D-02 2.178021676D-06
-7.824003460D-11 1.109909620D-15                 4.579268340D+06-1.752716908D+03
Sr+               Moore,1971. Gordon,1999.
 3 g 1/98 SR  1.00E  -1.00    0.00    0.00    0.00 0   87.6194514     716166.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 1.127287678D+01-1.346951870D-01 2.500651495D+00-1.635163061D-06 2.249493149D-09
-1.610827539D-12 4.698612333D-16                 8.538981180D+04 6.247259240D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 3.145095058D+06-9.514756890D+03 1.350086948D+01-6.059717120D-03 1.594068746D-06
-1.718800946D-10 6.322256169D-15                 1.457991907D+05-7.236416930D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6197.428
 9.016769220D+08-6.244641660D+05 1.695763594D+02-2.154835606D-02 1.462482744D-06
-4.930465390D-11 6.505705019D-16                 4.966238870D+06-1.431844579D+03
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Appendix D (*continued*)

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SrBr              Gurvich,1996a pt1 p522 pt2 p402.
 3 tpis96 SR  1.00BR  1.00     0.00     0.00     0.00 0  167.5240000      -63917.678
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10107.122
-7.549812420D+02-7.359532010D+01 4.828035810D+00-7.160584650D-04 1.028527433D-06
-6.888370720D-10 1.880257878D-13                 -8.686168450D+03 4.151153090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10107.122
 3.009976114D+06-9.193192240D+03 1.526033745D+01-6.009253950D-03 1.692611858D-06
-2.039438429D-10 8.807775840D-15                  4.922806130D+04-7.068253830D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10107.122
 2.274974243D+08-1.566004653D+05 4.234598410D+01-3.477076740D-03 1.358747452D-07
-2.623018618D-12 1.969298231D-17                  1.221445664D+06-3.265840740D+02
SrBr2             Gurvich,1996a pt1 p524 pt2 p404.
 2 tpis96 SR  1.00BR  2.00     0.00     0.00     0.00 0  247.4280000      -406725.851
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16334.649
-4.632458660D+03-7.244938640D+01 7.800217160D+00-6.772125310D-04 8.537780240D-07
-5.632351740D-10 1.510568795D-13                 -5.082238330D+04-5.285074760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16334.649
-1.186173059D+04-1.404383013D+00 7.501215570D+00-5.415983190D-07 1.296969275D-10
-1.580911652D-14 7.681582270D-19                 -5.118575210D+04-3.552037110D+00
SrCL              Gurvich,1996a pt1 p515 pt2 p398.
 3 tpis96 SR  1.00CL  1.00     0.00     0.00     0.00 0  123.0730000      -127867.882
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9800.118
 3.555346320D+03-1.729385697D+02 5.213451020D+00-1.542910668D-03 2.025835568D-06
-1.327076633D-09 3.547175960D-13                 -1.588288066D+04 4.818144784D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9800.118
 2.070217324D+06-6.199891730D+03 1.150315072D+01-3.675685460D-03 9.461732350D-07
-9.203765750D-11 2.707242192D-15                  2.271471632D+04-4.561058514D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9800.118
 1.382269500D+08-9.659524410D+04 2.600419230D+01-1.405193291D-03 2.007238545D-08
 7.119698480D-13-2.001316762D-17                  7.447979070D+05-1.876849167D+02
SrCL+             Gurvich,1996a pt1 p516 pt2 p399.
 3 g 8/98 SR  1.00CL  1.00E  -1.00     0.00     0.00 0  123.0724514      408112.162
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9582.762
 1.689043529D+03-1.749284676D+02 5.065328640D+00-9.857327840D-04 1.071655138D-06
-5.988127130D-10 1.395650932D-13                  4.861190260D+04 2.492001711D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9582.762
-2.132475783D+04-4.057948270D+00 4.503149390D+00 3.826202380D-05 2.676951510D-09
 5.667610500D-14 1.613288103D-18                  4.769326030D+04 3.637722496D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9582.762
-1.041313813D+04-7.208302400D+00 4.501589780D+00 3.937923600D-05 2.394465390D-09
 9.062292570D-14 4.723672450D-21                  4.772357520D+04 3.647375336D+00
SrCL2             Gurvich,1996a pt1 p520 pt2 p401.
 2 tpis96 SR  1.00CL  2.00     0.00     0.00     0.00 0  158.5260000      -484813.902
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14416.098
 1.913170011D+03-2.681156951D+02 8.081334300D+00-2.393329295D-03 2.976397494D-06
-1.943902862D-09 5.174307710D-13                 -5.910111850D+04-8.457827543D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14416.098
-2.592716099D+04-5.263785850D+00 7.004475240D+00-1.970397814D-06 4.679671200D-10
-5.670215880D-14 2.742892387D-18                 -6.045399530D+04-2.192202775D+00
SrF               Gurvich,1996a pt1 p507 pt2 p394.
 3 tpis96 SR  1.00F   1.00     0.00     0.00     0.00 0  106.6184032      -303552.788
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9283.112
 2.725008615D+04-4.850019720D+02 6.112697200D+00-3.008469209D-03 3.368465800D-06
-1.987813072D-09 4.884161090D-13                 -3.536890390D+04-6.683739180D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9283.112
 8.702340490D+05-2.589818770D+03 7.200264220D+00-1.173446296D-03 1.996165066D-07
 1.103842667D-11-2.343183859D-15                 -2.133671699D+04-1.667390309D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9283.112
-3.448093370D+07 2.208058158D+04-5.125719860D+00 2.209099383D-03-1.551627196D-07
 5.125524390D-12-6.680071600D-17                 -2.048593542D+05 7.995585500D+01
SrF+              Gurvich,1996a pt1 p511 pt2 p395.
 3 g 8/98 SR  1.00F   1.00E  -1.00     0.00     0.00 0  106.6178546      209468.312
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9106.812
 4.009624200D+04-5.944946080D+02 6.182330330D+00-2.716159750D-03 2.641369127D-06
-1.383123292D-09 3.052935853D-13                  2.697149351D+04-8.313659450D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9106.812
-4.752082060D+04-2.526802345D+01 4.519295280D+00 2.556426750D-05 3.382541830D-09
-1.511394636D-13 9.537491180D-18                  2.383861417D+04 1.892197325D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9106.812
-2.403608095D+03-3.242568700D+01 4.507124800D+00 3.261116540D-05 1.672393446D-09
 5.130259820D-14 2.102366585D-20                  2.392692006D+04 1.974517090D+00
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SrF2              Gurvich,1996a pt1 p514 pt2 p397.
 2 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 0  125.6168064     -784793.795
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13269.601
 4.170759650D+04-8.500132410D+02 1.002806064D+01-6.098485190D-03 7.056261330D-06
-4.359374310D-09 1.111308310D-12                -9.217859850D+04-2.325100053D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13269.601
-6.126265430D+04-1.964060822D+01 7.015557750D+00-6.512526780D-06 1.490473613D-09
-1.756437040D-13 8.317093850D-18                -9.656701250D+04-5.402308760D+00
SrH               Gurvich,1996a pt1 p499 pt2 p388.
 2 tpis96 SR  1.00H   1.00    0.00    0.00    0.00 0   88.6279400      219227.105
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8723.105
-4.317796890D+04 7.676429700D+02-1.594398638D+00 1.500711077D-02-1.826296898D-05
 1.136757659D-08-2.855588359D-12                 2.179685693D+04 3.324674230D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8723.105
-2.269825428D+05 1.345209458D+03 1.152194421D+00 3.109555289D-03-1.188080968D-06
 2.073091147D-10-1.300839287D-14                 1.735547062D+04 2.112916944D+01
SrI               Gurvich,1996a pt1 p526 pt2 p405.
 3 tpis96 SR  1.00I   1.00    0.00    0.00    0.00 0  214.5244700      -7851.676
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10283.124
-2.467498501D+03-2.535495809D+01 4.603298480D+00-1.613676212D-04 2.694294049D-07
-1.564795762D-10 3.826482280D-14                -2.175538291D+03 6.411481880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10283.124
 2.201136857D+06-7.082230700D+03 1.332597928D+01-5.305864420D-03 1.636071150D-06
-2.205540591D-10 1.078496824D-14                 4.219077170D+04-5.530833200D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10283.124
 1.557303348D+08-1.150787674D+05 3.550520760D+01-3.375329300D-03 1.695651221D-07
-4.438653930D-12 4.852777450D-17                 8.917357880D+05-2.613917335D+02
SrI2              Gurvich,1996a pt1 p528 pt2 p407.
 2 tpis96 SR  1.00I   2.00    0.00    0.00    0.00 0  341.4289400     -278218.842
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16701.658
-4.391849690D+03-3.757267350D+01 7.656993500D+00-3.561721300D-04 4.508689010D-07
-2.983230473D-10 8.018658660D-14                -3.553303460D+04-2.598281578D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16701.658
-8.090381920D+03-7.348263230D-01 7.500640060D+00-2.863515042D-07 6.876556970D-11
-8.398807360D-15 4.086968160D-19                -3.572106420D+04-1.693119087D+00
SrO               Gurvich,1996a pt1 p495 pt2 p384.
 3 tpis96 SR  1.00O   1.00    0.00    0.00    0.00 0  103.6194000     -14207.691
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9040.109
 4.224891670D+04-5.913517870D+02 5.964363000D+00-2.105712736D-03 2.028373972D-06
-1.197885492D-09 3.466289920D-13                 1.018053721D+02-7.511427470D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9040.109
-5.172933050D+07 1.510821000D+05-1.614513515D+02 8.516051790D-02-2.091669402D-05
 2.452307103D-09-1.108841292D-13                -9.687829520D+05 1.197846971D+03
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9040.109
 1.988729112D+08-9.438733680D+04 2.862378041D+01-2.923338947D-03 1.808436182D-07
-5.719087480D-12 7.320935570D-17                 7.583246290D+05-2.033702568D+02
SrO+              Gurvich,1996a pt1 p497 pt2 p386. Partridge,1986.
 3 g 8/98 SR  1.00O   1.00E  -1.00    0.00    0.00 0  103.6188514      630053.722
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10104.122
 4.618674160D+04-4.604560920D+02 5.605360720D+00-1.511707524D-03 1.328692506D-06
-6.244610540D-10 1.274632229D-13                 7.694140460D+04-3.377441410D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10104.122
 1.035147885D+06-3.339081120D+03 8.520055290D+00-2.340803237D-03 7.338594440D-07
-1.031868417D-10 5.087079240D-15                 9.540749060D+04-2.491223445D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10104.122
-6.910421610D+07 1.253686165D+04 9.522159370D+00-1.279343636D-03 8.998760920D-08
-2.931863956D-12 3.752244570D-17                -5.778506890D+04-3.231958760D+01
SrOH              Gurvich,1996a pt1 p502 pt2 p390.
 2 tpis96 SR  1.00O   1.00H   1.00    0.00    0.00 0  104.6273400     -194085.726
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11046.666
 4.640006560D+04-9.938685540D+02 9.784948960D+00-5.774377620D-03 5.126164110D-06
-1.833418356D-09 1.926013410D-13                -2.022721196D+04-2.740670981D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11046.666
 2.545648379D+06-7.416195980D+03 1.381956204D+01-3.096481934D-03 7.723894210D-07
-7.921280320D-11 2.740829111D-15                 2.231302058D+04-6.148781130D+01
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SrOH+              Gurvich,1996a pt1 p503 pt2 p391.
 2 tpis96 SR  1.00O   1.00H   1.00E  -1.00    0.00 0  104.6267914     310169.605
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11104.569
 3.857366940D+04-9.030242330D+02 9.451103250D+00-5.042516280D-03 4.190101890D-06
-1.196920603D-09 1.606318743D-14                 3.995067720D+04-2.601486110D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11104.569
 8.679695660D+05-2.340609538D+03 7.976829750D+00 1.023752569D-04-6.286032330D-08
 1.024851502D-11-5.723683920D-16                 5.073157720D+04-2.027046917D+01
Sr(OH)2            Gurvich,1996a pt1 p506 pt2 p393.
 2 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 0  121.6346800    -596694.573
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17011.921
 7.205090300D+04-1.789465226D+03 1.729429139D+01-1.169280781D-02 1.106702894D-05
-4.490146090D-09 6.603997460D-13                -6.605394040D+04-6.388681220D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17011.921
 1.750013518D+06-4.681601500D+03 1.395548402D+01 2.035019560D-04-1.253496115D-07
 2.044549432D-11-1.142004855D-15                -4.427170240D+04-5.051456850D+01
SrS                Gurvich,1996a pt1 p529 pt2 p409.
 2 tpis96 SR  1.00S   1.00    0.00    0.00    0.00 0  119.6850000     104351.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9536.115
 1.256440807D+04-3.150436559D+02 5.721722510D+00-2.630479718D-03 3.384699750D-06
-2.296256846D-09 6.512086680D-13                 1.277295160D+04-3.693874943D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9536.115
-1.379432947D+07 3.921331580D+04-3.602866380D+01 1.818513386D-02-3.275858160D-06
 2.324312746D-10-3.614555700D-15                -2.410246179D+05 2.991679642D+02
Sr2                Gurvich,1996a pt1 p491 pt2 p382.
 2 tpis96 SR  2.00    0.00    0.00    0.00    0.00 0  175.2400000     307570.337
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11365.137
-1.108859753D+05 5.927604010D+02 8.439688550D+00-2.652801112D-02 4.435825970D-05
-3.399915490D-08 9.965546680D-12                 3.157615033D+04-7.033966650D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11365.137
 2.098445682D+05 1.038650130D+02 2.309332330D+00 1.330517507D-04-4.426433390D-08
 6.711419150D-12-3.374128000D-16                 3.636642690D+04 2.168088517D+01
Ta                 Hf:Gurvich,1982 p85. Moore,1971. Gordon,1999.
 3 g 7/97 TA  1.00    0.00    0.00    0.00    0.00 0  180.9479000     782518.638
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6199.638
-1.150907339D+04 4.780730430D+01 3.185588390D+00-5.366528160D-03 1.288379705D-05
-1.045798666D-08 3.050617695D-12                 9.299797630D+04 5.336056610D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6199.638
 1.689726898D+06-5.986854660D+03 9.565039670D+00-2.511649459D-03 6.443031170D-07
-7.189237250D-11 3.113352070D-15                 1.306710983D+05-4.335096270D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6199.638
-8.413419560D+08 6.381509040D+05-1.856031850D+02 2.797353600D-02-2.073321805D-06
 7.397299170D-11-1.017863944D-15                -4.836410620D+06 1.607007750D+03
Ta+                Moore,1971. Gordon,1999.
 3 g 7/97 TA  1.00E  -1.00    0.00    0.00    0.00 0  180.9473514    1549679.335
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6337.835
 2.869712865D+05-3.084920994D+03 1.430679704D+01-1.984772164D-02 1.951445133D-05
-8.970946030D-09 1.501974665D-12                 2.013828712D+05-6.306427830D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6337.835
 3.656142130D+06-1.254073524D+04 1.865022579D+01-7.943274660D-03 2.151786937D-06
-2.816764844D-10 1.413722944D-14                 2.636876455D+05-1.065864286D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6337.835
 3.724273560D+07-3.405709310D+04 1.630056321D+01-2.064987830D-03 1.616826024D-07
-5.752060330D-12 7.636581870D-17                 4.405115500D+05-1.040237652D+02
Ta-                Hotop,1985. Gordon,1999.
 3 g 9/97 TA  1.00E   1.00    0.00    0.00    0.00 0  180.9484486     745469.429
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6416.129
 1.873982301D+05-1.681268679D+03 6.480040150D+00-2.254355782D-04 2.028434876D-06
-4.679801430D-09 1.997027996D-12                 9.793496020D+04-2.049618155D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6416.129
-4.235467480D+06 1.101056361D+04-4.736911070D+00 2.503562129D-03-4.821851690D-07
 4.886408030D-11-2.030547835D-15                 1.574699408D+04 6.491802700D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6416.129
 4.149884030D+05 1.227972146D+03 2.209211582D+00 3.401090760D-05-2.136872502D-09
 6.906775410D-14-9.017779200D-19                 8.249065600D+04 1.195636187D+01
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TaCL5             Chase,1998 p923.
 2 j12/74 TA  1.00CL  5.00    0.00    0.00    0.00 0  358.2129000    -764835.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26869.100
 6.306483290D+04-1.771221442D+03 2.255083356D+01-1.360238041D-02 1.613009806D-05
-1.016307761D-08 2.631917453D-12                 -8.792737110D+04-8.097864282D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26869.100
-1.426444545D+05-3.894340320D+01 1.603142370D+01-1.333676355D-05 3.084307611D-09
-3.663930060D-13 1.745841795D-17                 -9.701297170D+04-4.256986372D+01
TaO               Gurvich,1982 pt1 p86 pt2 p89.
 3 tpis89 TA  1.00O   1.00    0.00    0.00    0.00 0  196.9473000     242534.705
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8766.105
-1.395738049D+04 3.945236990D+02-6.301696410D-02 1.308595441D-02-1.862339730D-05
 1.366155583D-08-3.924551230D-12                  2.645195419D+04 2.741671469D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8766.105
 6.106591120D+06-1.984135246D+04 2.815797433D+01-1.330045882D-02 3.876807490D-06
-5.068872770D-10 2.443666035D-14                  1.525814433D+05-1.658307106D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8766.105
-1.076924766D+08 1.287348862D+04 1.361132509D+01-1.443306356D-03 9.697469230D-08
-3.170023830D-12 4.113579900D-17                 -1.302536682D+05-6.687940680D+01
TaO2              Gurvich,1982 pt1 p89 pt2 p91.
 2 tpis82 TA  1.00O   2.00    0.00    0.00    0.00 0  212.9467000    -173662.006
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10699.099
 1.516356303D+04 7.058414760D+01 6.918516990D-01 2.020605733D-02-2.928317413D-05
 2.081417374D-08-5.751106690D-12                 -2.212199468D+04 2.484662500D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10699.099
 1.297565964D+06-4.149217430D+03 1.041680373D+01-1.045478838D-03 2.754904271D-07
-3.297043130D-11 1.356249074D-15                  3.418985670D+03-3.392642790D+01
Ti                Hf:Cox,1989. Sugar,1985. Gordon,1999.
 3 g 7/97 TI  1.00    0.00    0.00    0.00    0.00 0   47.8670000     473000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7539.141
-4.570179400D+04 6.608092020D+02 4.295257490D-01 3.615029910D-03-3.549792810D-06
 1.759952494D-09-3.052720871D-13                  5.270947930D+04 2.026149738D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7539.141
-1.704786714D+05 1.073852803D+03 1.181955014D+00 2.245246352D-04 3.091697848D-07
-5.740027280D-11 2.927371014D-15                  4.978069910D+04 1.740431368D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7539.141
 1.152797766D+09-7.222408380D+05 1.777167465D+02-2.008059096D-02 1.221052354D-06
-3.811452080D-11 4.798092423D-16                  5.772614540D+06-1.518080466D+03
Ti+               Sugar,1985. Gordon,1999.
 3 g 7/97 TI  1.00E  -1.00    0.00    0.00    0.00 0   47.8664514    1137624.029
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7899.829
 1.707457044D+05-1.727524602D+03 9.615885330D+00-1.089655060D-02 8.201809650D-06
-2.871464413D-09 3.420382976D-13                  1.447897558D+05-3.463143660D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7899.829
-7.685463080D+05 2.545868100D+03 3.423862780D-01 7.099901360D-04 2.706231875D-08
-2.371660100D-11 1.895443077D-15                  1.198821489D+05 2.484799150D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7899.829
 3.918035620D+07-2.534581605D+04 9.586759720D+00-7.584155410D-04 4.432999350D-08
-8.442571760D-13-4.517128089D-19                  3.344440620D+05-5.220026270D+01
Ti-               Hotop,1985. Gordon,1999.
 3 g 9/97 TI  1.00E   1.00    0.00    0.00    0.00 0   47.8675486     459203.814
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7562.614
-3.006484990D+03 2.040911689D+02 1.822638976D+00 1.245254812D-03-1.309239865D-06
 7.372143220D-10-1.724319779D-13                  5.346772050D+04 1.205926588D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7562.614
 2.341117640D+04 2.580413872D+00 2.497754577D+00 9.769072040D-07-2.280024955D-10
 2.717202291D-14-1.295670294D-18                  5.454662180D+04 7.999823950D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7562.614
 1.417514172D+04 5.638799640D+00 2.498751709D+00 1.426579908D-07-8.889194940D-12
 2.867172222D-16-3.746329300D-21                  5.451843520D+04 7.994109450D+00
TiCL              Chase,1998 p808.
 2 j12/68 TI  1.00CL  1.00    0.00    0.00    0.00 0   83.3200000     150850.926
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9680.626
-1.714177839D+04 3.103259047D+02 8.920935980D-01 1.383436793D-02-1.885370354D-05
 1.212085912D-08-3.032162427D-12                  1.558066453D+04 2.244778384D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9680.626
-9.633225420D+05 2.868829781D+03 1.973820676D+00 1.752668011D-03-4.255434360D-07
 5.049103400D-11-2.304720715D-15                 -1.811011561D+03 2.319450287D+01
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TiCL2             Chase,1998 p866.
 2 j12/68 TI  1.00CL  2.00    0.00    0.00    0.00 0  118.7730000    -237230.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13545.270
 1.324354656D+04-5.762829320D+02 9.640047290D+00-4.475120950D-03 5.398794870D-06
-3.525800490D-09 9.746004550D-13                -2.792066683D+04-2.218347625D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13545.270
-3.190012950D+06 1.015763826D+04-4.840794770D+00 6.822006340D-03-1.700753270D-06
 2.118106588D-10-1.041245457D-14                -9.480982980D+04 7.823195948D+01
TiCL3             Chase,1998 p887.
 2 j12/68 TI  1.00CL  3.00    0.00    0.00    0.00 0  154.2260000    -539320.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15374.947
 1.243282268D+05-2.320728253D+03 1.779895274D+01-1.160889348D-02 1.006643154D-05
-4.811940690D-09 1.006186828D-12                -5.609602510D+04-6.732754065D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15374.947
-9.408792310D+04-1.255351109D+02 1.066923972D+01-2.637456897D-04 7.959169350D-08
-1.176740054D-11 6.416223480D-16                -6.769114680D+04-2.369164216D+01
TiCL4             Chase,1998 p906.
 2 j12/67 TI  1.00CL  4.00    0.00    0.00    0.00 0  189.6790000    -763160.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21613.541
 8.187196800D+04-1.758323850D+03 1.892512121D+01-1.133495876D-02 1.251952037D-05
-7.422681330D-09 1.825440187D-12                -8.672923110D+04-6.769594291D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21613.541
-1.432562278D+05-4.316774850D+01 1.303337752D+01-1.371365738D-05 3.093403483D-09
-3.604245160D-13 1.691384523D-17                -9.588947000D+04-3.247541011D+01
TiO               Gurvich,1982 pt1 p99 pt2 p101.
 3 tpis89 TI  1.00O   1.00    0.00    0.00    0.00 0   63.8664000     49503.615
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9593.115
-1.168152460D+04 4.542565650D+02-1.139144613D-01 1.275432333D-02-1.727656935D-05
 1.187369403D-08-3.236579370D-12                 2.924306353D+03 2.702903947D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9593.115
 2.330644030D+06-7.415793860D+03 1.281799311D+01-4.344555950D-03 1.186303111D-06
-1.367644275D-10 5.703212250D-15                 5.144841360D+04-5.793994240D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9593.115
 1.660288147D+08-1.051853502D+05 2.749141313D+01-1.681501753D-03 4.884078370D-08
-4.721389750D-13-2.405919722D-18                 8.399156070D+05-2.030813444D+02
TiO+              Gurvich,1982 pt1 p104 pt2 p103.
 3 tpis82 TI  1.00O   1.00E  -1.00    0.00    0.00 0   63.8658514     685321.011
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9213.111
 3.691256250D+04-1.492825538D+02 2.624977257D+00 5.818627130D-03-7.529662110D-06
 4.744154350D-09-1.186916989D-12                 8.241551170D+04 1.095428726D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9213.111
 3.421329530D+05-2.161851060D+03 8.025175660D+00-2.708700692D-03 1.004583805D-06
-1.505766850D-10 8.045658110D-15                 9.362646990D+04-2.261587887D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9213.111
 6.877707550D+07-4.060032000D+04 1.371193858D+01-6.905832140D-04 2.394468882D-08
-4.056406410D-13 2.475735466D-18                 4.034409840D+05-8.020740780D+01
TiOCL             Chase,1998 p796.
 2 j 9/63 TI  1.00O   1.00CL  1.00    0.00    0.00 0   99.3194000    -244262.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12142.701
 3.545856510D+04-6.295287140D+02 7.370176300D+00 3.302019140D-03-6.121458750D-06
 4.735880250D-09-1.374690357D-12                -2.797087903D+04-1.294470159D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12142.701
-1.273059873D+05-1.111118850D+02 7.582888080D+00-3.312871800D-05 7.314014090D-09
-8.378822260D-13 3.879275060D-17                -3.139356857D+04-1.247104274D+01
TiOCL2            Chase,1998 p843.
 2 j 9/63 TI  1.00O   1.00CL  2.00    0.00    0.00 0  134.7724000    -545552.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16710.010
 3.289052460D+04-7.389188590D+02 1.055976857D+01 1.577742341D-03-3.907182100D-06
 3.290576530D-09-9.949471750D-13                -6.448410700D+04-2.417469934D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16710.010
-1.322951633D+05-9.691212050D+01 1.007240769D+01-2.897248531D-05 6.401775040D-09
-7.338452600D-13 3.399282670D-17                -6.847409640D+04-1.975043469D+01
TiO2              Chase,1998 p1762 12/73. Jacox,1998.
 2 g10/99 TI  1.00O   2.00    0.00    0.00    0.00 0   79.8658000    -305430.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11351.690
-1.710545601D+03 2.721435528D+02 5.961378960D-01 1.925463599D-02-2.665500165D-05
 1.811109197D-08-4.876710470D-12                -3.912241770D+04 2.408605889D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11351.690
 1.546299764D+05-1.046256880D+03 7.788985830D+00-1.546805714D-04-7.059935950D-08
 3.100244802D-11-2.494725430D-15                -3.266336750D+04-1.591534660D+01
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U                Gurvich,1982 pt1 p184 pt2 p201. Blaise,1976.
 3 g 7/00 U   1.00    0.00    0.00    0.00    0.00 0  238.0289100     535000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6499.294
 6.965737750D+04-1.070351517D+03 8.075842310D+00-1.060034069D-02 9.256548010D-06
-3.219899760D-09 4.058048809D-13                 6.866513700D+04-2.240521678D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6499.294
-4.092498960D+06 1.274888349D+04-1.218707506D+01 7.258105680D-03-7.787775070D-07
-3.844353850D-11 7.066508567D-15                -1.699372664D+04 1.155026301D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6499.294
-2.424676814D+08 1.022495503D+05-2.321762289D+00-7.433177460D-04 9.674993970D-08
-4.159452280D-12 6.313829223D-17                -8.137559280D+05 7.333489176D+01
UF               Gurvich,1982 pt1 p202 pt2 p224.
 3 tpis82 U   1.00F   1.00    0.00    0.00    0.00 0  257.0273132     -49250.737
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9387.063
 1.725533463D+05-1.698985561D+03 5.902926430D+00 1.841977309D-02-4.633174310D-05
 4.376657200D-08-1.451876566D-11                 2.086455917D+03-1.186592944D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9387.063
-5.325439370D+06 1.533967086D+04-1.175044398D+01 9.647210930D-03-2.498778190D-06
 3.155572896D-10-1.544694839D-14                -1.057196525D+05 1.220828149D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9387.063
 2.021978468D+08-1.196840152D+05 3.263355240D+01-2.553105588D-03 1.191730174D-07
-2.677714445D-12 2.360089903D-17                 9.473656850D+05-2.396788565D+02
UF+              Gurvich,1982 pt1 p203 pt2 p226.
 3 tpis82 U   1.00F   1.00E  -1.00    0.00    0.00 0  257.0267646     557058.967
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9499.367
 1.622640597D+06-1.917326611D+04 8.759461220D+01-1.699915707D-01 1.861251683D-04
-1.036176702D-07 2.324287412D-11                 1.616709643D+05-4.806891249D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9499.367
 5.395091840D+05-2.923962095D+03 1.008511948D+01-2.425945123D-03 5.928725480D-07
-6.795845540D-11 3.152666445D-15                 8.267291220D+04-3.307089704D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9499.367
 5.357726300D+07-1.105107069D+04 1.891324705D+00 1.246403421D-03-1.128508026D-07
 4.314527550D-12-6.027569830D-17                 1.776673362D+05 2.409952635D+01
UF-              Gurvich,1982 pt1 p204 pt2 p228.
 3 g12/99 U   1.00F   1.00E   1.00    0.00    0.00 0  257.0278618    -155679.193
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9156.007
 3.692327860D+03-1.491979606D+02 4.033988520D+00 2.857429445D-03-5.171702560D-06
 3.985379110D-09-9.470355440D-13                -1.915281695D+04 6.059243838D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9156.007
-4.311143560D+06 1.974817938D+04-2.760304763D+01 2.276806261D-02-6.888741720D-06
 9.483511060D-10-4.910688100D-14                -1.380801290D+05 2.240758537D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9156.007
-3.090384299D+08 1.824173856D+05-3.570033800D+01 4.596835280D-03-2.809511961D-07
 9.028550240D-12-1.169274383D-16                -1.475954920D+06 3.592431751D+02
UF2              Gurvich,1982 pt1 p205 pt2 p230.
 3 tpis82 U   1.00F   2.00    0.00    0.00    0.00 0  276.0257164     -535036.715
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15152.392
-3.882492020D+04 4.454930860D+02 4.718009190D+00 1.648911480D-03 8.696243010D-06
-1.207439921D-08 4.536793910D-12                -6.855329330D+04 1.159725423D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15152.392
-4.716776820D+05 3.224236860D+02 8.214090630D+00-1.407413780D-04 6.541178050D-09
 1.818915497D-12-2.287963719D-16                -6.995235050D+04-9.648963156D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15152.392
 3.833722170D+06-5.166288400D+03 1.000042588D+01-3.502166850D-04 1.973413760D-08
-5.613962470D-13 6.472362570D-18                -2.897767010D+04-2.492966720D+01
UF2+             Gurvich,1982 pt1 p207 pt2 p232.
 3 tpis82 U   1.00F   2.00E  -1.00    0.00    0.00 0  276.0251678      70445.527
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14437.127
 5.439010160D+03-1.507096256D+02 6.873485190D+00 1.530973969D-03-3.316694310D-06
 2.949453335D-09-8.281706540D-13                 7.256014910D+03-2.205491833D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14437.127
-3.779149610D+06 1.298737504D+04-1.027930641D+01 1.048838051D-02-2.651047812D-06
 3.116973593D-10-1.417216291D-14                -7.433440200D+04 1.189131079D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14437.127
-9.003702250D+07 4.886273610D+04-2.192209667D-01 6.378651730D-04-3.372669300D-08
 9.777729090D-13-1.189890068D-17                -3.936562000D+05 6.595164355D+01
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UF2-              Gurvich,1982 pt1 p208 pt2 p234.
 3 tpis82 U   1.00F   2.00E   1.00     0.00     0.00 0  276.0262650    -678233.195
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13153.339
 8.060491730D+05-9.404254660D+03 4.448392770D+01-6.868558770D-02 6.777809920D-05
-3.338827680D-08 6.604851620D-12                -3.603306130D+04-2.261594249D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13153.339
 1.038231855D+07-2.840113518D+04 3.498533370D+01-1.053216396D-02 1.924620470D-06
-1.698749570D-10 5.709858890D-15                 1.001572794D+05-2.094039075D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13153.339
-5.046229980D+07 3.524957180D+04-8.601752150D-01 8.947422820D-04-5.540675440D-08
 1.776021844D-12-2.307535574D-17                -3.584621110D+05 6.877566575D+01
UF3               Gurvich,1982 pt1 p210 pt2 p237.
 3 tpis82 U   1.00F   3.00     0.00     0.00     0.00 0  295.0241196   -1060958.597
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18643.063
 3.071027207D+04-6.340789470D+02 1.114030799D+01-2.937554125D-04-1.865390371D-06
 2.371819470D-09-7.446754070D-13                -1.271838141D+05-2.348962529D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18643.063
-3.828876420D+06 1.296891783D+04-7.265554290D+00 1.048289752D-02-2.649840687D-06
 3.115594509D-10-1.416579400D-14                -2.113615913D+05 1.054464687D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18643.063
-9.007768940D+07 4.885212250D+04 2.783068500D+00 6.376088800D-04-3.371098360D-08
 9.772726250D-13-1.189242739D-17                -5.307242640D+05 5.256841035D+01
UF3+              Gurvich,1982 pt1 p211 pt2 p239.
 3 tpis82 U   1.00F   3.00E  -1.00     0.00     0.00 0  295.0235710    -284745.430
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18658.870
-3.984155890D+05 3.480892440D+03-2.519603507D+00 2.283749282D-02-2.168844780D-05
 1.111265790D-08-2.350882012D-12                -5.550889200D+04 5.853815975D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18658.870
-1.196316388D+06 3.972785070D+03 4.535907110D+00 4.133416150D-03-1.097960689D-06
 1.319641252D-10-6.101129180D-15                -6.199541740D+04 2.137623045D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18658.870
-4.490516590D+07 2.285903928D+04 7.869516510D+00 1.274792626D-04-5.228047920D-09
 1.360286305D-13-1.645113815D-18                -2.269266296D+05 6.797911871D+00
UF3-              Gurvich,1982 pt1 p212 pt2 p241.
 3 tpis82 U   1.00F   3.00E   1.00     0.00     0.00 0  295.0246682   -1186440.771
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19358.329
-2.315187300D+05 2.534197822D+03-3.180714590D+00 2.932741422D-02-2.856912260D-05
 1.345804152D-08-2.465442912D-12                -1.580387746D+05 5.973605435D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19358.329
-1.910053149D+05-5.069181310D+02 1.181482258D+01-1.711879404D-04-9.384839180D-08
 2.242009537D-11-1.428195280D-15                -1.438628681D+05-2.774680411D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19358.329
-1.944714123D+07 1.429185303D+04 7.239366640D+00 2.897026663D-04-1.704156160D-08
 5.276150470D-13-6.688352280D-18                -2.573053031D+05 1.122428161D+01
UF4               Gurvich,1982 pt1 p215 pt2 p244.
 3 tpis82 U   1.00F   4.00     0.00     0.00     0.00 0  314.0225228   -1606157.418
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21892.582
-5.007852380D+04-9.693493550D+02 2.069596355D+01-2.564852637D-02 4.195860120D-05
-3.201013390D-08 9.422076860D-12                -1.931626334D+05-7.172362935D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21892.582
-1.230291173D+06 3.876463790D+03 7.621625910D+00 4.094525220D-03-1.088530094D-06
 1.308042117D-10-6.044390870D-15                -2.214142920D+05 6.270300658D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21892.582
-4.422199930D+07 2.244095755D+04 1.096208609D+01 1.168958941D-04-4.568843620D-09
 1.147904592D-13-1.368068374D-18                -3.836270440D+05-8.486934342D+00
UF4+              Gurvich,1982 pt1 p216 pt2 p246.
 3 tpis82 U   1.00F   4.00E  -1.00     0.00     0.00 0  314.0219742    -641539.484
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20313.316
 3.848956330D+04-1.343282151D+03 1.646334809D+01-7.196079860D-03 1.147165041D-05
-8.705877980D-09 2.501076195D-12                -7.405048200D+04-5.295285535D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20313.316
-1.617630159D+06 3.765934770D+03 9.166138530D+00 2.426641067D-03-5.695320300D-07
 6.021096600D-11-2.438874329D-15                -1.061910645D+05-4.162641042D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20313.316
-2.790280948D+07 1.464555692D+04 1.168522991D+01 5.249951330D-05-1.762380856D-10
-5.000071600D-14 1.088450028D-18                -2.028630553D+05-1.708462849D+01
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UF4-              Gurvich,1982 pt1 p217 pt2 p248.
 3 tpis82 U   1.00F   4.00E   1.00    0.00    0.00 0  314.0230714   -1728334.866
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21876.775
 7.203179690D+04-1.374343862D+03 1.640877729D+01-4.363066270D-03 2.460407959D-06
-1.498144731D-10-1.239417075D-13                -2.045174023D+05-5.172250795D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21876.775
-4.639200110D+06 1.626824426D+04-9.595291050D+00 1.441556535D-02-4.008173850D-06
 5.140230790D-10-2.511687821D-14                -3.125140933D+05 1.274038784D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21876.775
-1.308421305D+08 8.061319300D+04-3.939161520D+00 1.853747295D-03-1.116700599D-07
 3.508474880D-12-4.490622440D-17                -8.552752700D+05 1.210372085D+02
UF5               Gurvich,1982 pt1 p219 pt2 p251.
 3 tpis82 U   1.00F   5.00    0.00    0.00    0.00 0  333.0209260   -1949823.884
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23602.882
 1.615769193D+05-2.976611537D+03 2.537542420D+01-1.930105670D-02 2.561852107D-05
-1.747402896D-08 4.732059380D-12                -2.239089616D+05-1.024264836D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23602.882
-1.695373880D+06 3.735425350D+03 1.218748040D+01 2.418608203D-03-5.678526160D-07
 6.002765610D-11-2.430740809D-15                -2.645107342D+05-1.883137475D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23602.882
-2.820007103D+07 1.475725044D+04 1.466020135D+01 5.538728810D-05-3.572588510D-10
-4.414506670D-14 1.011890437D-18                -3.622893270D+05-3.137230618D+01
UF5+              Gurvich,1982 pt1 p220 pt2 p253.
 3 tpis82 U   1.00F   5.00E  -1.00    0.00    0.00 0  333.0203774    -853617.242
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23612.158
 1.626519713D+05-2.915370389D+03 2.436168077D+01-1.382199656D-02 1.339849041D-05
-7.078572690D-09 1.573404040D-12                -9.226404850D+04-9.830243935D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23612.158
-2.628478263D+05-1.174047323D+02 1.608988291D+01-3.665516710D-05 8.221494970D-09
-9.537160520D-13 4.460145080D-17                -1.076293931D+05-4.763374165D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23612.158
-4.772763820D+04-1.534892435D+02 1.603372733D+01-3.833472040D-06 2.377658266D-10
-7.638474870D-15 9.946126940D-20                -1.071959701D+05-4.725516365D+01
UF5-              Gurvich,1982 pt1 p221 pt2 p255.
 3 tpis82 U   1.00F   5.00E   1.00    0.00    0.00 0  333.0214746   -2289431.237
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25192.963
-3.142130934D+05 2.020611008D+03 7.508491820D+00 1.640034396D-02-1.562795472D-05
 7.990246010D-09-1.671674534D-12                -2.907647496D+05 4.690020575D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25192.963
-1.331518187D+06 3.905516860D+03 1.058727667D+01 4.112507270D-03-1.093277930D-06
 1.314215436D-10-6.075778270D-15                -3.049506955D+05-7.977511665D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25192.963
-4.492648300D+07 2.277621599D+04 1.388769935D+01 1.254140874D-04-5.100027930D-09
 1.319174409D-13-1.591595740D-18                -4.696748520D+05-2.232978306D+01
UF6               Gurvich,1982 pt1 p223 pt2 p257.
 3 tpis82 U   1.00F   6.00    0.00    0.00    0.00 0  352.0193292   -2148641.648
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26623.352
 1.915674060D+05-3.426391610D+03 2.800395890D+01-1.326392086D-02 1.107123764D-05
-4.821754110D-09 8.325132450D-13                -2.461045194D+05-1.211612947D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26623.352
-3.409027920D+05-1.458950046D+02 1.910902533D+01-4.358451130D-05 9.617604660D-09
-1.100915551D-12 5.092645080D-17                -2.643645561D+05-6.579130396D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26623.352
-2.639780713D+05-8.680089820D+01 1.901877513D+01-2.107561344D-06 1.295346553D-10
-4.136090060D-15 5.365237680D-20                -2.646640074D+05-6.513581536D+01
UF6-              Gurvich,1982 pt1 p224 pt2 p258.
 3 tpis82 U   1.00F   6.00E   1.00    0.00    0.00 0  352.0198778   -2691306.150
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27730.597
 1.569230858D+05-3.027279940D+03 2.701442427D+01-1.136860992D-02 8.298576160D-06
-2.582889593D-09 2.790817248D-13                -3.135307376D+05-1.128934794D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27730.597
 2.699676848D+06-6.574459670D+03 2.241731997D+01 6.057799710D-04-4.517491710D-07
 7.821820470D-11-4.560334720D-15                -2.855667984D+05-9.182896336D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27730.597
-7.865804610D+07 4.174825500D+04 1.201141201D+01 6.958372750D-04-4.049760430D-08
 1.262006447D-12-1.620083625D-17                -6.704395130D+05 1.746878673D+00
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Appendix D (*continued*)

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UO                Gurvich,1982 pt1 p186 pt2 p205.
 3 tpis82 U   1.000O   1.00    0.00    0.00    0.00 0  254.0283100      30488.589
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9538.289
 1.007249615D+06-1.287190666D+04 5.993123920D+01-1.003445164D-01 8.529345550D-05
-2.634105066D-08-5.350649790D-13                 6.627442520D+04-3.226786779D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9538.289
-2.458660003D+06 3.942652160D+03 5.016030720D+00-5.450639470D-04 2.096321351D-07
-2.654652526D-11 1.361108472D-15                -2.665149645D+04 5.580598689D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9538.289
 1.643829702D+08-6.893889290D+04 1.274655043D+01 3.898071910D-04-8.455141670D-08
 4.053706450D-12-6.354764880D-17                 5.854610850D+05-7.355640184D+01
UO+               Gurvich,1982 pt1 p189 pt2 p207.
 3 tpis82 U   1.000O   1.00E -1.00    0.00    0.00 0  254.0277614     580971.927
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8824.227
 1.562834007D+04-1.224921454D+02 3.324146160D+00 2.467496097D-03-6.851856740D-07
 5.552073190D-11-5.893012030D-14                 6.952999740D+04 9.583869879D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8824.227
-1.063714748D+05-1.793716133D+03 8.024449050D+00-1.565116442D-03 5.066033910D-07
-7.373977470D-11 4.074766430D-15                 7.789085840D+04-2.115284250D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8824.227
-4.623486280D+07 4.390299020D+04-9.206507600D+00 2.335209239D-03-1.678226513D-07
 5.653921370D-12-7.297202790D-17                -2.648708363D+05 1.200887991D+02
UOF               Gurvich,1982 pt1 p225 pt2 p259.
 2 tpis82 U   1.000O   1.00F   1.00    0.00    0.00 0  273.0267132     -542182.744
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14005.456
 3.861248470D+02 5.162286900D+01 4.888962520D+00 7.265633560D-03-1.134176875D-05
 8.509041750D-09-2.354655485D-12                -6.719813380D+04 8.269521875D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14005.456
-3.805936010D+06 1.295207909D+04-1.025373631D+01 1.047841671D-02-2.648894949D-06
 3.114551623D-10-1.416111895D-14                -1.478976701D+05 1.184570601D+02
UOF2              Gurvich,1982 pt1 p226 pt2 p261.
 2 tpis82 U   1.000O   1.00F   2.00    0.00    0.00 0  292.0251164    -1115510.264
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17816.436
-9.106618310D+04-1.014150169D+02 1.371057013D+01-1.659931694D-02 3.082352584D-05
-2.490530206D-08 7.580617640D-12                -1.374686016D+05-3.470029665D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17816.436
-1.198944060D+06 3.852173410D+03 4.639109750D+00 4.087738440D-03-1.087067018D-06
 1.306398384D-10-6.036901520D-15                -1.612637583D+05 2.018237189D+01
UOF3              Gurvich,1982 pt1 p229 pt2 p264.
 2 tpis82 U   1.000O   1.00F   3.00    0.00    0.00 0  311.0235196    -1510638.039
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19827.161
 1.249256374D+05-2.111719498D+03 1.844931536D+01-1.041493583D-02 1.469002962D-05
-1.049770051D-08 2.922353602D-12                -1.743844024D+05-6.649285435D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19827.161
-1.658296049D+06 3.714434680D+03 9.202425540D+00 2.412862293D-03-5.666241720D-07
 5.989062110D-11-2.424534810D-15                -2.105491714D+05-5.670532802D+00
UOF4              Gurvich,1982 pt1 p230 pt2 p265.
 2 tpis82 U   1.000O   1.00F   4.00    0.00    0.00 0  330.0219228    -1785611.531
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22742.734
 1.437164405D+05-2.496730363D+03 2.104827038D+01-4.692561330D-03 8.741718650D-07
 1.517555623D-09-7.768799740D-13                -2.061284178D+05-8.246219615D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22742.734
-2.996190288D+05-1.677276501D+02 1.612494871D+01-4.984414460D-05 1.098253497D-08
-1.255803231D-12 5.804480980D-17                -2.195459260D+05-5.024484645D+01
UO2               Gurvich,1982 pt1 p193 pt2 p211.
 3 tpis82 U   1.000O   2.00    0.00    0.00    0.00 0  270.0277100     -477819.903
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13460.097
-1.129650727D+05 4.270730270D+02 8.413694010D+00-9.764280000D-03 2.199903691D-05
-1.907665954D-08 6.029889910D-12                -6.251443300D+04-1.300704863D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13460.097
-1.190542635D+06 3.832186350D+03 2.153236312D+00 4.082351910D-03-1.085924847D-06
 1.305134065D-10-6.031215750D-15                -8.367618010D+04 2.590742388D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13460.097
-4.415894110D+07 2.241359238D+04 5.468051300D+00 1.162219348D-04-4.527223330D-09
 1.134573678D-13-1.350744532D-18                -2.459740375D+05 1.133700240D+01
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UO2+                Gurvich,1982 pt1 p194 pt2 p213.
 3 tpis82 U   1.000   2.00E  -1.00    0.00    0.00 0  270.0271614       51493.919
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11576.519
 4.488023380D+04-6.489236420D+02 6.874243560D+00 2.281949316D-03 1.859218752D-07
-1.849509036D-09 8.149965330D-13                 7.891740230D+03-1.028257233D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11576.519
-1.589957420D+06 3.657746070D+03 3.746785420D+00 2.394401448D-03-5.624101440D-07
 5.939451640D-11-2.401047056D-15                -2.048558817D+04 1.464015614D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11576.519
-2.778324150D+07 1.456161876D+04 6.203516610D+00 5.043474040D-05-4.877674180D-11
-5.408292310D-14 1.141506994D-18                -1.172230791D+05 2.164589095D+00
UO2-                Gurvich,1982 pt1 p195 pt2 p215.
 3 tpis82 U   1.000   2.00E   1.00    0.00    0.00 0  270.0282586     -573700.021
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13777.379
 6.341971310D+04-7.196118500D+02 8.308241620D+00 9.626455450D-04-3.583733980D-06
 3.473554580D-09-1.022793120D-12                -6.718169870D+04-1.606030120D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13777.379
-2.738251640D+05 3.228534420D+03-2.805114576D-01 6.607310710D-03-2.070291015D-06
 2.851708013D-10-1.466578192D-14                -8.893436180D+04 4.145760316D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13777.379
-1.053612192D+08 6.331803380D+04-5.853591580D+00 1.472289928D-03-8.933245500D-08
 2.824078529D-12-3.633249210D-17                -5.772299570D+05 1.092379584D+02
UO2F                Gurvich,1982 pt1 p226 pt2 p260.
 2 tpis82 U   1.000   2.00F   1.00    0.00    0.00 0  289.0261132     -997934.842
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15803.758
 8.321792390D+04-1.327082127D+03 1.240125390D+01-4.084151010D-03 7.331593480D-06
-5.987404880D-09 1.787869209D-12                -1.157526888D+05-3.415298625D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15803.758
-1.614277202D+06 3.712771860D+03 6.203308820D+00 2.412618055D-03-5.665888020D-07
 5.988823520D-11-2.424485602D-15                -1.478357384D+05 8.736139132D+00
UO2F2               Gurvich,1982 pt1 p228 pt2 p263.
 2 tpis82 U   1.000   2.00F   2.00    0.00    0.00 0  308.0245164    -1354232.027
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19067.973
 9.959874300D+04-1.530010701D+03 1.358992177D+01 5.370655800D-03-1.141444341D-05
 9.301197040D-09-2.781220538D-12                -1.580310734D+05-4.196260275D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19067.973
-2.636552036D+05-2.032835065D+02 1.315092994D+01-6.006486830D-05 1.321137913D-08
-1.508668985D-12 6.966182750D-17                -1.664444818D+05-3.566258175D+01
UO3                 Gurvich,1982 pt1 p197 pt2 p218.
 3 tpis82 U   1.000   3.00    0.00    0.00    0.00 0  286.0271100     -799239.411
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15144.745
 6.637677040D+04-7.582646580D+02 7.112844710D+00 1.322149697D-02-2.106191042D-05
 1.545856318D-08-4.378566290D-12                -9.413369350D+04-8.588030428D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15144.745
-1.097362721D+06 2.808784061D+03 5.966121470D+00 2.861871152D-03-1.052843810D-06
 1.849985929D-10-1.102849619D-14                -1.173360017D+05 6.672828312D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15144.745
 1.632929098D+09-9.419553920D+05 2.142384145D+02-2.094922993D-02 1.131511326D-06
-3.129107183D-11 3.504914590D-16                 7.448065370D+06-1.824526663D+03
UO3-                Gurvich,1982 pt1 p198 pt2 p220.
 3 tpis82 U   1.000   3.00E   1.00    0.00    0.00 0  286.0276586    -1305154.518
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15427.082
 1.000143902D+05-1.448443754D+03 1.217532415D+01-2.944956748D-03 5.675228000D-06
-4.916710420D-09 1.525185713D-12                -1.519253376D+05-3.471731375D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15427.082
-1.632938634D+06 3.667495410D+03 6.240030650D+00 2.396952522D-03-5.629490230D-07
 5.945413130D-11-2.403730982D-15                -1.845927385D+05 7.032059012D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15427.082
-2.781940595D+07 1.456116475D+04 8.703650860D+00 5.041649230D-05-4.751131470D-11
-5.412647410D-14 1.142098108D-18                -2.812591514D+05-5.495926098D+00
V                   Hf:Gurvich,1982 p59. Sugar,1985. Gordon,1999.
 3 g 7/97 V   1.00    0.00    0.00    0.00    0.00 0   50.9415000      517267.064
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7907.064
-5.535376020D+04 5.593338510D+02 2.675543482D+00-6.243049630D-03 1.565902337D-05
-1.372845314D-08 4.168388810D-12                 5.820664360D+04 9.524567490D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7907.064
 1.200390300D+06-5.027005300D+03 1.058830594D+01-5.044326100D-03 1.488547375D-06
-1.785922508D-10 8.113013866D-15                 9.170740910D+04-4.768336320D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7907.064
 2.456040166D+09-1.339992028D+06 2.781039851D+02-2.638937359D-02 1.303527149D-06
-3.214680330D-11 3.099999094D-16                 1.087152043D+07-2.439954380D+03
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V+                Sugar,1985. Gordon,1999.
 3 g 7/97 V   1.00E  -1.00    0.00    0.00    0.00 0   50.9409514    1173745.411
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7897.811
 7.568834460D+04-8.415273820D+02 7.559232710D+00-1.441722656D-02 2.038356397D-05
-1.289073883D-08 3.065656561D-12                 1.444478191D+05-1.991067645D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7897.811
 2.347072054D+06-9.021197190D+03 1.477349798D+01-6.891896880D-03 1.968884877D-06
-2.539798544D-10 1.226783122D-14                 1.958351444D+05-7.855592930D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7897.811
 2.516527258D+08-1.866476656D+05 5.633587110D+01-7.198536950D-03 5.074401490D-07
-1.699749225D-11 2.157800037D-16                 1.585980536D+06-4.512822600D+02
V-                Hotop,1985. Gordon,1999.
 3 g 9/97 V   1.00E   1.00    0.00    0.00    0.00 0   50.9420486     460386.063
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7878.263
-3.799273560D+03 2.313840448D+02 1.725608190D+00 1.429275357D-03-1.506038188D-06
 8.491815170D-10-1.987980413D-13                 5.347402920D+04 1.261900982D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7878.263
 2.600100430D+04 2.096334097D+00 2.498006548D+00 8.991278840D-07-2.139749508D-10
 2.581021334D-14-1.240812796D-18                 5.470007080D+04 7.977900240D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7878.263
 1.601102910D+04 5.820974900D+00 2.498705489D+00 1.484212570D-07-9.272956840D-12
 2.997799727D-16-3.924862230D-21                 5.466692550D+04 7.974557420D+00
VCL4              Nagarajan,1963. Creighton,1966. Blankenship,1962.
 2 g10/00 V   1.00CL  4.00    0.00    0.00    0.00 0  192.7535000    -527058.480
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21783.098
 7.719834710D+04-1.702854040D+03 1.882697965D+01-1.130896832D-02 1.266950765D-05
-7.625019340D-09 1.907582465D-12                -5.863748540D+04-6.559171106D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21783.098
-1.717776251D+06 4.550441050D+03 8.164464800D+00 2.224875998D-03-4.094111780D-07
 3.271787500D-11-8.858690800D-16                -9.690620060D+04 4.348293098D+00
VN                Chase,1998 p1616.
 2 j12/73 V   1.00N   1.00    0.00    0.00    0.00 0   64.9482000     523000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8799.744
-1.581737285D+04 4.868165420D+02-1.045200388D+00 1.685261043D-02-2.334616543D-05
 1.588710050D-08-4.279080880D-12                 5.981481400D+04 3.144995263D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8799.744
 1.018619667D+06-3.932305570D+03 9.856823610D+00-3.289221710D-03 1.005181767D-06
-1.243211436D-10 5.486776560D-15                 8.557318340D+04-3.552830762D+01
VO                Gurvich,1982 pt1 p62 pt2 p64.
 3 tpis89 V   1.00O   1.00    0.00    0.00    0.00 0   66.9409000     148582.706
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8773.106
-1.311619784D+04 3.747816970D+02 9.300834860D-02 1.244977714D-02-1.688540028D-05
 1.142443381D-08-3.040589320D-12                 1.523789920D+04 2.536811755D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8773.106
 2.986190283D+06-1.011344974D+04 1.718161749D+01-7.876705030D-03 2.562279547D-06
-3.547400350D-10 1.770268056D-14                 7.961254880D+04-8.789993010D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8773.106
 1.004530292D+08-9.008780230D+04 3.186107720D+01-2.862639937D-03 1.440482244D-07
-3.802861470D-12 4.195092660D-17                 7.011401290D+05-2.336810859D+02
VO2               Gurvich,1982 pt1 p64 pt2 p66.
 2 tpis82 V   1.00O   2.00    0.00    0.00    0.00 0   82.9403000    -232697.655
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10622.449
-6.678585860D+03 3.911597580D+02-1.028549847D+00 2.401523419D-02-3.337378810D-05
 2.283623543D-08-6.199143100D-12                -3.074609276D+04 3.277912380D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10622.449
 1.210632401D+05-1.627832993D+03 9.252713100D+00-1.572703139D-03 5.231430160D-07
-6.476071140D-11 2.847226026D-15                -2.097306345D+04-2.547380687D+01
V4O10             Gurvich,1982 pt1 p69 pt2 p70.
 2 g10/99 V   4.00O  10.00    0.00    0.00    0.00 0  363.7600000   -2825164.486
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         36796.033
 3.385739160D+05-5.353929260D+03 2.993220131D+01 5.818836520D-02-9.696340160D-05
 7.274756990D-08-2.091628357D-11                -3.189349370D+05-1.466398396D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         36796.033
-1.360273270D+06-1.341692860D+03 4.099138590D+01-3.932265530D-04 8.628494120D-08
-9.835944090D-12 4.535637290D-16                -3.484616120D+05-1.907911348D+02
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Appendix D (*continued*)

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W                 Hf:Gurvich,1982 p42. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 4/98 W   1.00    0.00    0.00    0.00    0.00 0  183.8400000     851243.526
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6216.526
 1.595223922D+05-2.673843928D+03 2.060469727D+01-6.252315230D-02 1.105654838D-04
-8.453511610D-08 2.336187771D-11                 1.139648616D+05-9.011836900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6216.526
-8.048745960D+06 1.465700424D+04-2.508531501D-01-2.596486992D-03 1.409225475D-06
-2.233011706D-10 1.262640862D-14                -3.091130919D+03 3.955822190D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6216.526
 1.421636486D+09-4.325365550D+05-8.841615070D+00 1.645538940D-02-1.908373835D-06
 8.530482890D-11-1.360501851D-15                 3.994798750D+06-1.266418236D+01
W+                Moore,1971. Gordon,1999.
 3 g 7/97 W   1.00E -1.00    0.00    0.00    0.00 0  183.8394514    1627840.965
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6221.265
-1.969284929D+05 2.670137332D+03-1.131686913D+01 3.308183730D-02-3.629035500D-05
 2.066142971D-08-4.808285562D-12                 1.820950862D+05 8.552104480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6221.265
 6.387743400D+06-2.061811463D+04 2.759291576D+01-1.244535845D-02 3.271200490D-06
-4.065463720D-10 1.912595872D-14                 3.245174430D+05-1.716919194D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6221.265
 6.839559150D+07-8.981711810D+04 3.845720800D+01-5.465752290D-03 4.024981150D-07
-1.342970538D-11 1.667637540D-16                 8.546932820D+05-2.892805521D+02
W-                Hotop,1985. Gordon,1999.
 3 g 1/99 W   1.00E   1.00    0.00    0.00    0.00 0  183.8405486     766391.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 9.142981370D+04 8.461169670D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 9.142981370D+04 8.461169670D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 9.142981370D+04 8.461169670D+00
WCL6              Chase,1998 p935.
 2 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 0  396.5580000    -493712.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         30790.955
 3.339391670D+04-1.697366080D+03 2.560612352D+01-1.425247881D-02 1.739682668D-05
-1.120537864D-08 2.951522890D-12                -5.673059240D+04-9.741466299D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         30790.955
-1.516735473D+05-3.451379250D+01 1.902867176D+01-1.242486969D-05 2.917675103D-09
-3.505981440D-13 1.685355887D-17                -6.535779790D+04-5.894914959D+01
WO                Gurvich,1982 pt1 p43 pt2 p47.
 3 tpis82 W   1.00O   1.00    0.00    0.00    0.00 0  199.8394000     401735.711
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9259.111
-1.933758411D+04 4.936690840D+02-4.116148220D-01 1.307976507D-02-1.689145619D-05
 1.092748066D-08-2.820593541D-12                 4.511017900D+04 3.002592661D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9259.111
 1.262156956D+06-4.177263120D+03 9.358286470D+00-2.887612220D-03 8.893933960D-07
-8.955318700D-11 2.504359614D-15                 7.313380640D+04-3.144882290D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9259.111
 1.942009403D+08-1.501316158D+05 4.237023540D+01-3.309676390D-03 1.396809578D-07
-3.039263166D-12 2.703787815D-17                 1.214349290D+06-3.296819210D+02
WOCL4             Chase,1998 p900.
 2 j 3/67 W   1.00O   1.00CL  4.00    0.00    0.00 0  341.6514000     -573493.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22271.379
 2.658812693D+04-9.336913240D+02 1.321377385D+01 1.270930811D-02-1.964716509D-05
 1.405106974D-08-3.899382140D-12                -6.792290790D+04-3.594869683D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22271.379
-3.049028285D+05-3.539425860D+02 1.626432703D+01-1.058245461D-04 2.340548846D-08
-2.685852021D-12 1.245412684D-16                -7.272546740D+04-4.991761253D+01
WO2               Gurvich,1982 pt1 p47 pt2 p50.
 2 tpis82 W   1.00O   2.00    0.00    0.00    0.00 0  215.8388000      29061.744
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10714.848
 3.120918919D+03 2.413883468D+02-3.024119184D-01 2.324333417D-02-3.378812680D-05
 2.380934019D-08-6.421592880D-12                 1.442005265D+03 2.957655179D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10714.848
-7.537406680D+05 3.204643050D+03 6.701965600D-01 4.488238870D-03-8.858328460D-07
 6.245171750D-11-9.046613900D-16                -1.769420230D+04 3.405724010D+01
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WO2CL2            Chase,1998 p849.
 2 j 3/67 W   1.000   2.00CL  2.00     0.00     0.00 0  286.7448000    -671532.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19503.817
 4.300154480D+02-2.438547856D+02 7.976306990D+00 1.715005722D-02-2.487975176D-05
 1.737644163D-08-4.771928400D-12                 -8.232812400D+04-7.844771421D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19503.817
-2.404791730D+05-3.068379644D+02 1.322814502D+01-9.100220710D-05 2.006581020D-08
-2.296837607D-12 1.062829386D-16                 -8.367493060D+04-3.491556626D+01
WO3               Gurvich,1982 pt1 p50 pt2 p52.
 2 tpis82 W   1.000   3.00    0.00     0.00     0.00 0  231.8382000    -319725.213
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13267.943
 7.262461460D+03 3.429391090D+01 1.573061955D+00 2.754971099D-02-3.994827310D-05
 2.809371537D-08-7.777545730D-12                 -4.001733270D+04 1.857409963D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13267.943
 1.732203640D+06-6.284719780D+03 1.681358864D+01-3.472089360D-03 8.079935800D-07
-6.589378720D-11 1.142928957D-15                 -2.473075565D+03-7.407474090D+01
WO3-              Gurvich,1982 pt1 p51 pt2 p53.
 2 tpis82 W   1.000   3.00E   1.00     0.00     0.00 0  231.8387486    -650475.961
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13714.639
 1.630999684D+05-1.967609682D+03 1.201970914D+01 1.681260779D-03-5.859360060D-06
 5.028616330D-09-1.434012198D-12                 -7.009203990D+04-3.936901040D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13714.639
 4.637832510D+05-1.347089334D+03 9.773637560D+00 1.071395459D-03-3.842403660D-07
 5.737531900D-11-3.157605982D-15                 -7.239515570D+04-2.391116343D+01
(WO3)2            Gurvich,1982 pt1 p52 pt2 p54.
 2 tpis82 W   2.000   6.00    0.00     0.00     0.00 0  463.6764000   -1210443.298
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25543.014
 8.088414510D+04-9.060340790D+02 7.601575390D+00 5.241008510D-02-7.922356390D-05
 5.708640180D-08-1.606775042D-11                 -1.441496996D+05-1.093524051D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25543.014
-6.674072430D+05-7.032518360D+02 2.251617461D+01-2.035473339D-04 4.444320340D-08
-5.045188080D-12 2.318375739D-16                 -1.502699479D+05-8.613988980D+01
(WO3)3            Gurvich,1982 pt1 p53 pt2 p55.
 2 tpis82 W   3.000   9.00    0.00     0.00     0.00 0  695.5146000   -2013291.101
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          40688.367
 3.485390010D+04-1.933496319D+02 8.206544780D+00 8.599515510D-02-1.257565252D-04
 8.891567220D-08-2.471213564D-11                 -2.462453469D+05-5.657325260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          40688.367
-9.450263310D+05-1.133837222D+03 3.483479230D+01-3.301361100D-04 7.226602130D-08
-8.221581630D-12 3.785050840D-16                 -2.488486308D+05-1.441551053D+02
(WO3)4            Gurvich,1982 pt1 p54 pt2 p56.
 2 tpis82 W   4.000  12.00    0.00     0.00     0.00 0  927.3528000   -2817433.885
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          54538.739
 1.388606167D+04 2.287518563D+02 8.662370000D+00 1.219700696D-01-1.770499494D-04
 1.246790033D-07-3.456182860D-11                 -3.467839600D+05-3.603937290D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          54538.739
-1.277530217D+06-1.566538532D+03 4.715363520D+01-4.563263220D-04 9.990758360D-08
-1.136816181D-11 5.234399340D-16                 -3.477418470D+05-2.051588395D+02
(WO3)5            Gurvich,1982 pt1 p56 pt2 p57.
 2 tpis82 W   5.000  15.00    0.00     0.00     0.00 0 1159.1910000   -3551492.326
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          68473.453
 1.497576743D+04 2.719999782D+02 1.138626896D+01 1.523302100D-01-2.211447753D-04
 1.557377753D-07-4.317244680D-11                 -4.371424320D+05-1.441643481D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          68473.453
-1.600667953D+06-1.958437864D+03 5.944227390D+01-5.705105630D-04 1.249090916D-07
-1.421320416D-11 6.544458260D-16                 -4.384095860D+05-2.660238838D+02
Xe                Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.
 3 g 1/99 XE  1.00    0.00    0.00     0.00     0.00 0  131.2930000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.453750000D+02 6.164454205D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.025226680D+03-1.209507521D+01 2.514153347D+00-8.248102080D-06 2.530232618D-09
-3.892333230D-13 2.360439138D-17                 -6.685800730D+02 6.063710715D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 2.540397456D+08-1.105373774D+05 1.382644099D+01 1.500614606D-03-3.935359030D-07
 2.765790584D-11-5.943990574D-16                 9.285443830D+05-1.109834556D+02
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Xe+                Moore,1971. Moore,1970a. Gordon,1999.
 3 g 3/97 XE  1.00E  -1.00    0.00    0.00    0.00 0  131.2924514    1176552.232
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 1.002923620D+02-1.218753648D+00 2.506016493D+00-1.547411334D-05 2.191372741D-08
-1.623684074D-11 4.929132670D-15                 1.407665368D+05 7.516712465D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.241683887D+04-1.500654643D+02 2.964678293D+00-4.693396660D-04 1.959138719D-07
-3.037761925D-11 1.637361082D-15                 1.414966808D+05 4.565685735D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.562275878D+08 1.570476914D+05-3.635537230D+01 5.019392580D-03-3.438107240D-07
 1.140544651D-11-1.295661530D-16                -1.103556546D+06 3.436188813D+02
Zn                 Hf:Cox,1989. Sugar,1995. Gordon,1999.
 3 g 6/97 ZN  1.00    0.00    0.00    0.00    0.00 0   65.3900000     130400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.493805072D+04 5.118861010D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-1.755591489D+05 4.984139240D+02 1.969386292D+00 2.608808787D-04-5.627195080D-08
 2.723336049D-12 4.266685808D-16                 1.173773458D+04 8.961085650D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-2.087287962D+08 1.578178131D+05-3.622033110D+01 3.345230020D-03-8.567422720D-09
-7.122544740D-12 1.691187274D-16                -1.217847671D+06 3.459439960D+02
Zn+                Sugar,1995. Gordon,1999.
 3 g 6/97 ZN  1.00E  -1.00    0.00    0.00    0.00 0   65.3894514    1043000.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21                 1.246979918D+05 5.811995500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-3.436179460D+05 9.567355240D+02 1.511478952D+00 4.613467960D-04-8.786800980D-08
 7.558567780D-13 1.168827311D-15                 1.185321933D+05 1.300742670D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
-3.011747676D+09 2.074729347D+06-5.589526960D+02 7.501396440D-02-5.136763100D-06
 1.741662147D-10-2.323920111D-15                -1.609057856D+07 4.824788010D+03
Zr                 Hf:Gurvich,1982. Moore,1971. Hackett,1986. Gordon,1999.
 3 g 1/98 ZR  1.00    0.00    0.00    0.00    0.00 0   91.2240000     599318.611
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6815.611
 6.715899960D+04-9.435981740D+02 6.359756180D+00-9.790119730D-04-7.608224150D-06
 9.308717430D-09-3.124675586D-12                 7.588019470D+04-1.665770522D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6815.611
 6.006771840D+06-1.566960605D+04 1.796982350D+01-6.763409650D-03 1.733678968D-06
-2.064699786D-10 9.334092610D-15                 1.734636249D+05-1.051117377D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6815.611
 5.207701380D+08-2.825652444D+05 6.077054350D+01-5.081211410D-03 2.345845819D-07
-6.237212120D-12 8.010718759D-17                 2.351487351D+06-5.093183060D+02
Zr+                Moore,1971. Moore,1970a. Gordon,1999.
 3 g 1/98 ZR  1.00E  -1.00    0.00    0.00    0.00 0   91.2234514    1246246.292
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7471.892
 1.739842193D+05-2.224598466D+03 1.400787829D+01-2.378785396D-02 2.641058912D-05
-1.442565487D-08 3.135982142D-12                 1.598210714D+05-5.816728810D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7471.892
 7.298137160D+05-2.017117556D+03 5.037498300D+00-5.503371950D-04 1.023753499D-07
-1.261537793D-11 7.092401042D-16                 1.620884945D+05-9.820640860D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7471.892
-2.294818875D+07 1.860972745D+04-1.661509984D+00 6.020341290D-04-3.930742580D-08
 1.543806931D-12-2.618341088D-17                 4.907298890D+03 4.642130480D+01
Zr-                Hotop,1985. Gordon,1999.
 3 g 2/98 ZR  1.00E   1.00    0.00    0.00    0.00 0   91.2245486     552952.398
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7749.498
 3.046662367D+04-8.074277210D+02 9.213006110D+00-1.614342054D-02 1.908653551D-05
-1.138888914D-08 2.745019116D-12                 6.903034030D+04-2.862644371D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7749.498
 8.471861160D+04 3.175439340D+02 2.251491246D+00 1.018645389D-04-2.285208242D-08
 2.647293502D-12-1.235813604D-16                 6.422337600D+04 1.081261057D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7749.498
-4.386641560D+05 3.768748730D+02 2.417088403D+00 9.411538660D-06-5.824251210D-10
 1.866281342D-14-2.423724320D-19                 6.334701050D+04 9.677778690D+00
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ZrN                Chase,1998 p1620.
 2 j 6/63 ZR  1.00N   1.00     0.00     0.00     0.00 0  105.2307000      713372.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8862.870
 2.259109156D+04-1.802590198D+02 3.130058377D+00 5.427709280D-03-8.264614840D-06
 5.958438220D-09-1.670274535D-12                 8.578881490D+04 8.470724780D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8862.870
-7.255790890D+04-8.126796600D+01 4.559924400D+00 1.291161650D-05 5.203830770D-09
-5.927436670D-13 2.731548854D-17                 8.468648390D+04 1.493633264D+00
ZrO                Gurvich,1982 pt1 p118 pt2 p118.
 3 tpis82 ZR  1.00O   1.00     0.00     0.00     0.00 0  107.2234000       83922.708
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8970.108
-5.091761400D+05 8.652770090D+03-5.294740150D+01 1.728961761D-01-2.457230895D-04
 1.672135156D-07-4.423012380D-11                -3.095129818D+04 3.132576719D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8970.108
 4.648098310D+05 3.442314470D+02 4.815779180D+00-4.660633140D-04 2.140489079D-07
-2.054364483D-11 4.084667760D-16                 7.317340700D+03 1.502933548D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8970.108
 1.343456923D+08-7.851088360D+04 1.981614195D+01-8.027211020D-04 2.522081797D-09
 7.959625600D-13-1.684162816D-17                 6.406670590D+05-1.358472283D+02
ZrO+               Gurvich,1982 pt1 p122 pt2 p120.
 3 tpis82 ZR  1.00O   1.00E  -1.00     0.00     0.00 0  107.2228514      720614.114
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9464.114
 1.032911549D+04 7.304661220D+01 2.606345299D+00 5.099300290D-03-6.250338760D-06
 3.797460020D-09-9.198416900D-13                 8.533233780D+04 1.267311019D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9464.114
-4.937166560D+05 6.699900760D+02 4.575353470D+00-6.923237900D-04 4.280600940D-07
-7.547660220D-11 4.414279860D-15                 8.018880660D+04 2.928943704D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9464.114
 4.389941590D+07-2.084044161D+04 8.167126240D+00-5.668596640D-05-8.861355220D-09
 4.773106180D-13-7.435660480D-18                 2.554517908D+05-3.127152387D+01
ZrO2               Gurvich,1982 pt1 p125. Chase,1998 p1772 12/65.
 2 g10/99 ZR  1.00O   2.00     0.00     0.00     0.00 0  123.2228000     -317042.737
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12008.263
 3.637649000D+04-2.620658297D+02 3.692866870D+00 1.214524156D-02-1.822445342D-05
 1.299215204D-08-3.615900110D-12                -3.801990880D+04 8.290857600D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12008.263
 2.854363887D+06-8.738589890D+03 1.621315114D+01-4.417922830D-03 8.959096920D-07
-4.054667110D-11-2.147732083D-15                 1.527510023D+04-7.481995490D+01
Ag(cr)             Cubic. Ref-Elm. Cox,1989 p228.
 1 coda89 AG  1.00    0.00     0.00     0.00     0.00 1  107.8682000          0.000
    200.000   1235.0807 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5745.000
-7.099236470D+04 7.254788020D+02 1.066518380D-01 5.529541550D-03-4.425590850D-06
 2.091668120D-09-3.888924460D-13                -4.614014260D+03 5.074216040D+00
Ag(L)              Liquid. Ref-Elm. Cox,1989 p228.
 1 coda89 AG  1.00    0.00     0.00     0.00     0.00 2  107.8682000          0.000
   1235.080   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5745.000
 0.000000000D+00 0.000000000D+00 4.017073770D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.672269970D+02-1.771527070D+01
AL(cr)             Cubic. Ref-Elm. Cox,1989 p217.
 1 coda89 AL  1.00    0.00     0.00     0.00     0.00 1   26.9815380          0.000
    200.000    933.6107 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4540.000
-6.251811430D+04 6.343934350D+02-7.131883820D-01 1.088725280D-02-1.458741820D-05
 9.961160880D-09-1.774928010D-12                -3.985439320D+03 6.561100200D+00
AL(L)              Liquid. Ref-Elm. Cox,1989 p217.
 1 coda89 AL  1.00    0.00     0.00     0.00     0.00 2   26.9815380          0.000
    933.610   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4540.000
 0.000000000D+00 0.000000000D+00 3.818625510D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.576323160D+01-1.752553420D+01
ALBr3(cr)          Monoclinic. Gurvich,1996a pt1 p187 pt2 p150.
 1 tpis96 AL  1.00BR  3.00     0.00     0.00     0.00 1  266.6935380     -511500.000
    200.000    371.1607 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21920.000
-1.907292099D+05 0.000000000D+00 2.665662652D+01-8.326099820D-02 1.395828123D-04
 0.000000000D+00 0.000000000D+00                -6.763881140D+04-1.126522667D+02
ALBr3(L)           Liquid. Gurvich,1996a pt1 p187 pt2 p150.
 1 tpis96 AL  1.00BR  3.00     0.00     0.00     0.00 2  266.6935380     -511500.000
    371.160   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21920.000
 0.000000000D+00 0.000000000D+00 1.503395871D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.481402080D+04-6.083617689D+01
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ALCL3(cr)          Monoclinic. Gurvich,1996a pt1 p172 pt2 p133.
 1 tpis96 AL  1.00CL  3.00    0.00    0.00    0.00 1  133.3405380    -705100.000
    200.000    465.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16980.000
-2.605551108D+05 2.535762396D+03-1.248379067D+00 2.465425813D-02-8.048550150D-06
 0.000000000D+00 0.000000000D+00                -1.007777032D+05 2.030375677D+01
ALCL3(L)           Liquid. Gurvich,1996a pt1 p172 pt2 p133.
 1 tpis96 AL  1.00CL  3.00    0.00    0.00    0.00 2  133.3405380    -705100.000
    465.700   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16980.000
 0.000000000D+00 0.000000000D+00 1.509409454D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.559022460D+04-6.519014639D+01
ALF3(II)           Hexagonal. Gurvich,1996a pt1 p156 pt2 p119.
 2 tpis96 AL  1.00F   3.00    0.00    0.00    0.00 1   83.9767476   -1510400.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11620.400
 0.000000000D+00 0.000000000D+00-2.444621150D+00 6.248607440D-02-8.043962500D-05
 0.000000000D+00 0.000000000D+00                -1.829961207D+05 6.871585170D+00
    298.150    728.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11620.400
 0.000000000D+00 0.000000000D+00-3.158574588D+00 7.101368571D-02-1.246540085D-04
 7.930377136D-08 0.000000000D+00                -1.829283321D+05 9.661469435D+00
ALF3(I)            Cubic. Gurvich,1996a pt1 p156 pt2 p119.
 1 tpis96 AL  1.00F   3.00    0.00    0.00    0.00 2   83.9767476   -1510400.000
    728.000   2100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11620.400
-1.060675855D+05 0.000000000D+00 1.114052422D+01 1.092668119D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.853502219D+05-5.651122021D+01
ALH3(a)            Alpha,hexagonal. Gurvich,1996a pt1 p144 pt2 p108.
 1 tpis96 AL  1.00H   3.00    0.00    0.00    0.00 1   30.0053580    -11400.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5440.000
 5.744612990D+05-7.649579650D+03 3.481355430D+01-4.495737990D-02 2.948551342D-05
 0.000000000D+00 0.000000000D+00                3.549793150D+04-2.050727589D+02
ALI3(cr)           Hexagonal. Gurvich,1996a pt1 p193 pt2 p155.
 1 tpis96 AL  1.00I   3.00    0.00    0.00    0.00 1  407.6949480    -302900.000
    298.150    461.4707 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22300.000
-3.486280460D+03 0.000000000D+00 8.644374370D+00 1.088065032D-02 5.040262220D-07
 0.000000000D+00 0.000000000D+00                -3.950736400D+04-2.968661932D+01
ALI3(L)            Liquid. Gurvich,1996a pt1 p193 pt2 p155.
 1 tpis96 AL  1.00I   3.00    0.00    0.00    0.00 2  407.6949480    -302900.000
    461.470   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22300.000
 0.000000000D+00 0.000000000D+00 1.455287203D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.913903150D+04-5.670488781D+01
ALN(cr)            Hexagonal. Gurvich,1996a pt1 p202 pt2 p163.
 2 tpis96 AL  1.00N   1.00    0.00    0.00    0.00 1   40.9882380    -319000.000
    100.000    300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          3870.000
 3.654741530D+03 0.000000000D+00-2.148600451D+00 2.744441314D-02-2.763366825D-05
 0.000000000D+00 0.000000000D+00                -3.868948290D+04 7.733969220D+00
    300.000   1800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          3870.000
-1.801549340D+05 0.000000000D+00 5.525280504D+00 4.025492783D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.063616530D+04-3.018829926D+01
ALN(L)             Liquid. Gurvich,1996a pt1 p202 pt2 p163.
 2 tpis96 AL  1.00N   1.00    0.00    0.00    0.00 3   40.9882380    -319000.000
   1800.000   2700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          3870.000
 0.000000000D+00 0.000000000D+00 4.491184688D+00 9.460569534D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.955518910D+04-2.338770283D+01
   2700.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          3870.000
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.755928440D+04-4.598731266D+01
AL(OH)3(a)         Gibbsite. Gurvich,1996a pt1 p150 pt2 p114.
 1 tpis96 AL  1.00O   3.00H   3.00    0.00    0.00 1   78.0035580   -1293500.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12460.000
-2.376748819D+04 9.289791210D+02-1.532337335D+01 1.307578268D-01-2.205157141D-04
 1.567014467D-07 0.000000000D+00                -1.605485750D+05 6.795129010D+01
AL2O3(a)           Alpha,corundum. Gurvich,1996a pt1 p134 pt2 p103.
 3 tpis96 AL  2.00O   3.00    0.00    0.00    0.00 1  101.9612760   -1675700.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10016.000
-5.391549970D+06 1.036676983D+05-8.173229150D+02 3.388258720D+00-7.512400360D-03
 8.659248820D-06-4.066085670D-09                -6.660134650D+05 4.235502230D+03
    500.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10016.000
-6.042087868D+05 0.000000000D+00 1.475480816D+01 8.272285438D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.079235447D+05-8.136029480D+01
   1200.000   2327.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10016.000
 0.000000000D+00 0.000000000D+00 1.293774378D+01 1.992781294D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.060787581D+05-6.966603728D+01
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AL2O3(L)          Liquid. Gurvich,1996a pt1 p134 pt2 p103.
 1 tpis96 AL  2.00O   3.00    0.00    0.00    0.00 3  101.9612760   -1675700.000
   2327.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10016.000
 0.000000000D+00 0.000000000D+00 1.959225499D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.027701571D+05-1.108590952D+02
AL2S3(a)          Hexagonal alpha. Gurvich,1996a pt1 p201 pt2 p162.
 2 tpis96 AL  2.00S   3.00    0.00    0.00    0.00 1  150.1580760    -648500.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18630.440
 0.000000000D+00 0.000000000D+00-1.347810098D+00 8.478152110D-02-1.270516814D-04
 0.000000000D+00 0.000000000D+00                -8.024014680D+04 2.103644584D+00
    298.150   1273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18630.440
-1.943109095D+05 0.000000000D+00 1.417618116D+01 2.164890054D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.297075040D+04-6.845362098D+01
AL2S3(b)          Rhombohedral gamma. Gurvich,1996a pt1 p201 pt2 p162.
 1 tpis96 AL  2.00S   3.00    0.00    0.00    0.00 3  150.1580760    -648500.000
   1273.000   1373.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18630.440
 0.000000000D+00 0.000000000D+00 1.683803375D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.445251510D+04-8.466769750D+01
AL2S3(L)          Liquid. Gurvich,1996a pt1 p201 pt2 p162.
 1 tpis96 AL  2.00S   3.00    0.00    0.00    0.00 4  150.1580760    -648500.000
   1373.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18630.440
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.114023330D+04-9.722848599D+01
AL2SiO5(an)       Andalusite. Chase,1998 p160.
 3 j 9/67 AL  2.00SI  1.00O   5.00    0.00    0.00 1  162.0455760   -2592072.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17093.000
-5.435020350D+05 8.364904470D+03-5.479541870D+01 2.421451459D-01-3.247828060D-04
 1.619746222D-07 0.000000000D+00                -3.531115760D+05 2.892220103D+02
    600.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17093.000
 9.635670330D+06-6.505315100D+04 1.886717981D+02-2.227599181D-01 1.677460173D-04
-6.532301110D-08 1.041420443D-11                 4.284683500D+04-1.170130476D+03
   1500.000   3000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17093.000
 5.600590290D+07-1.591905491D+05 2.058003747D+02-1.103017260D-01 3.860284650D-05
-6.943079960D-09 5.126291370D-13                 6.964365160D+05-1.424396263D+03
AL4C3(cr)         Hexagonal. Gurvich,1996a pt1 p207 pt2 p168.
 2 tpis96 AL  4.00C   3.00    0.00    0.00    0.00 1  143.9582520    -206900.000
    100.000    300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16470.000
 4.384127580D+03 0.000000000D+00-5.803779650D+00 1.009595640D-01-1.158851541D-04
 0.000000000D+00 0.000000000D+00                -2.660263745D+04 1.884004031D+01
    300.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16470.000
-4.483607573D+05 0.000000000D+00 1.788920814D+01 4.024290066D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.190056250D+04-9.494910735D+01
B(b)              Beta. Ref-Elm.  Chase,1998 p177-180. McBride,1993a.
 2 j 6/83 B   1.00    0.00    0.00    0.00    0.00 1   10.8110000          0.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1214.000
 2.598259342D+05-4.770773050D+03 3.464124480D+01-1.287342209D-01 2.897864235D-04
-3.307265950D-07 1.500151011D-10                 2.146946846D+04-1.830824723D+02
    600.000   2350.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1214.000
-8.697700220D+02-8.050405960D+02 4.079712880D+00-6.423381350D-04 4.846017800D-07
-1.252780673D-10 1.335923595D-14                 3.397919930D+03-2.505906587D+01
B(L)              Liquid. Ref-Elm.  Chase,1998 p177-180. McBride,1993a.
 1 j 6/83 B   1.00    0.00    0.00    0.00    0.00 2   10.8110000          0.000
   2350.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1214.000
 0.000000000D+00 0.000000000D+00 3.818625511D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.360603140D+03-2.073167308D+01
BN(cr)            Hexagonal. Gurvich,1996a pt1 p103 pt2 p82.
 2 tpis96 B   1.00N   1.00    0.00    0.00    0.00 1   24.8177000    -251000.000
    200.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         2628.425
 4.927312430D+05-6.086406850D+03 2.678226753D+01-4.529686640D-02 5.305526030D-05
-3.041114432D-08 6.795343860D-12                -2.413474891D+02-1.570534002D+02
   1200.000   3240.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         2628.425
-8.394039490D+05 0.000000000D+00 6.231256640D+00-1.258688680D-05 2.018144787D-09
 0.000000000D+00 0.000000000D+00                -3.427269230D+04-3.687260910D+01
BN(L)             Liquid. Gurvich,1996a pt1 p103 pt2 p82.
 1 tpis96 B   1.00N   1.00    0.00    0.00    0.00 2   24.8177000    -251000.000
   3240.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         2628.425
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.023409980D+04-4.862382389D+01
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B2O3(cr)          Hexagonal. Gurvich,1996a pt1 p21 pt2 p16.
 1 tpis96 B   2.00O   3.00    0.00    0.00    0.00 1   69.6202000   -1273500.000
    100.000    723.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9301.499
-5.595297380D+04 1.311214190D+03-1.178535942D+01 7.702795250D-02-9.740126500D-05
 4.692119720D-08 1.804813810D-12                 -1.599672923D+05 5.866759160D+01
B2O3(L)           Liquid. Gurvich,1996a pt1 p21 pt2 p16.
 1 tpis96 B   2.00O   3.00    0.00    0.00    0.00 2   69.6202000   -1273500.000
    723.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9301.499
 3.774124994D+05 0.000000000D+00 1.528015481D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.562115789D+05-8.056094941D+01
B2S3(cr)          Monoclinic. Gurvich,1996a pt1 p101 pt2 p80.
 1 tpis96 B   2.00S   3.00    0.00    0.00    0.00 1  117.8170000    -243000.000
    298.150    840.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17200.400
-9.430501617D+04 0.000000000D+00 1.190088171D+01 8.711277033D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.347775180D+04-5.890696350D+01
B2S3(L)           Liquid. Gurvich,1996a pt1 p101 pt2 p80.
 1 tpis96 B   2.00S   3.00    0.00    0.00    0.00 2  117.8170000    -243000.000
    840.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17200.400
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.921234633D+04-8.268126136D+01
B3O3H3(cr)        Chase,1998 p287.
 3 j 3/65 B   3.00H   3.00O   3.00    0.00    0.00 1   83.4550200   -1262313.000
    298.150    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-5.328545240D+05 3.767360370D+03 6.890276350D-01-4.217091030D-03 8.303566290D-05
-6.146021890D-08 0.000000000D+00                 -1.757027581D+05 2.395113516D+01
    700.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 5.084004120D+07-3.177180280D+05 8.113753320D+02-1.045412717D+00 7.976442970D-04
-3.265400500D-07 5.554759650D-11                 1.623716865D+06-5.113032450D+03
   1400.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-3.234845810D+08 1.232060747D+06-1.920881017D+03 1.628142178D+00-7.579315580D-04
 1.870131216D-07-1.915685535D-11                 -7.655560210D+06 1.307505171D+04
B4C(cr)           Hexagonal. Gurvich,1996a pt1 p111 pt2 p89
 2 tpis96 B   4.00C   1.00    0.00    0.00    0.00 1   55.2547000     -62000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5611.469
-3.582115390D+07 6.748884130D+05-5.160630080D+03 2.049973510D+01-4.453648770D-02
 5.049831300D-05-2.340979136D-08                 -3.040618105D+06 2.693617477D+04
    500.000   2743.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5611.469
-5.772904970D+05 0.000000000D+00 1.274373364D+01 5.718209610D-05 1.287030822D-06
 0.000000000D+00 0.000000000D+00                 -1.320621763D+04-7.266962500D+01
B4C(L)            Liquid. Chase,1998 pp556-8.
 1 j 6/83 B   4.00C   1.00    0.00    0.00    0.00 2   55.2547000     -62000.000
   2743.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5611.469
 0.000000000D+00 0.000000000D+00 1.635454164D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.250553215D+03-9.163227046D+01
Ba(cr)            Crystal. Ref-Elm. Alcock,1993.
 2 srd 93 BA  1.00    0.00    0.00    0.00    0.00 1  137.3270000             0.000
     80.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6906.992
-1.121413048D+03 0.000000000D+00 2.794031158D+00 3.089779193D-03-8.812305235D-06
 1.741533776D-08 0.000000000D+00                 -9.306838000D+02-9.109787138D+00
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6906.992
 0.000000000D+00 0.000000000D+00 2.773344430D+00 2.037522355D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.174338100D+02-8.909706262D+00
Ba(L)             Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 BA  1.00    0.00    0.00    0.00    0.00 2  137.3270000             0.000
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6906.992
 0.000000000D+00 0.000000000D+00 4.810866786D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.920623810D+02-2.000275711D+01
BaBr2(cr)         Rhombic. Gurvich,1996a pt1 p578 pt2 p438.
 1 tpis96 BA  1.00BR  2.00    0.00    0.00    0.00 1  297.1350000     -752000.000
    298.000   1130.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19000.460
-7.817658527D+03 0.000000000D+00 8.433088661D+00 2.644894287D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.310239840D+04-3.084013513D+01
BaBr2(L)          Liquid. Gurvich,1996a pt1 p578 pt2 p438.
 1 tpis96 BA  1.00BR  2.00    0.00    0.00    0.00 2  297.1350000     -752000.000
   1130.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19000.460
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.227494300D+04-5.391493900D+01
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BaCO3(a)          CrIII,rhombic. Gurvich,1996a pt1 p588 pt2 p446.
 2 tpis96 BA  1.00C   1.00O   3.00     0.00     0.00 1  197.3359000   -1214000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16510.460
-2.877181104D+07 5.413510470D+05-4.125297560D+03 1.638620098D+01-3.558188760D-02
 4.031953330D-05-1.867325900D-08                -2.581769925D+06 2.154826876D+04
    500.000   1083.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16510.460
-4.578261377D+05 0.000000000D+00 1.897622349D+01-1.614166078D-02 1.493894409D-05
 0.000000000D+00 0.000000000D+00                -1.526176829D+05-9.306389650D+01
BaCO3(b)          CrII,hexagonal. Gurvich,1996a pt1 p588 pt2 p446.
 1 tpis96 BA  1.00C   1.00O   3.00     0.00     0.00 3  197.3359000   -1214000.000
   1083.000   1233.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16510.460
 0.000000000D+00 0.000000000D+00 1.900292380D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.534042929D+05-9.996568172D+01
BaCO3(c)          CrI,cubic. Gurvich,1996a pt1 p588 pt2 p446.
 1 tpis96 BA  1.00C   1.00O   3.00     0.00     0.00 4  197.3359000   -1214000.000
   1233.000   1828.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16510.460
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.533520950D+05-1.013948007D+02
BaCO3(L)          Liquid. Gurvich,1996a pt1 p588 pt2 p446.
 1 tpis96 BA  1.00C   1.00O   3.00     0.00     0.00 5  197.3359000   -1214000.000
   1828.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16510.460
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.496405113D+05-1.032798247D+02
BaCL2(a)          CrII,rhombic. Gurvich,1996a pt1 p574 pt2 p435.
 2 tpis96 BA  1.00CL  2.00     0.00     0.00     0.00 1  208.2330000    -855200.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16700.460
-7.376444120D+04 1.806760784D+03-1.415837573D+01 1.391571933D-01-4.179089240D-04
 6.207438290D-07-3.577305500D-10                -1.127273901D+05 7.349900590D+01
    500.000   1198.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16700.460
 7.096028509D+02 0.000000000D+00 8.343245723D+00 2.300676769D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.054434434D+05-3.333989736D+01
BaCL2(b)          CrI,cubic. Gurvich,1996a pt1 p574 pt2 p435.
 1 tpis96 BA  1.00CL  2.00     0.00     0.00     0.00 3  208.2330000    -855200.000
   1198.000   1234.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16700.460
 0.000000000D+00 0.000000000D+00 1.575558872D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.105803253D+05-8.137880037D+01
BaCL2(L)          Liquid. Gurvich,1996a pt1 p574 pt2 p435.
 1 tpis96 BA  1.00CL  2.00     0.00     0.00     0.00 4  208.2330000    -855200.000
   1234.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16700.460
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.054088841D+05-6.099987667D+01
BaF2(a)           CrIII,cubic. Gurvich,1996a pt1 p567 pt2 p431.
 2 tpis96 BA  1.00F   2.00     0.00     0.00     0.00 1  175.3238064    -1206000.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14440.460
 1.441693954D+05-4.606283760D+03 5.412180390D+01-2.221460987D-01 5.733095130D-04
-7.321844990D-07 3.715051400D-10                -1.283756240D+05-2.649277473D+02
    500.000   1240.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14440.460
-2.180525371D+04 0.000000000D+00 7.730461567D+00 3.587703906D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.475854552D+05-3.364924914D+01
BaF2(b)           CrII. Gurvich,1996a pt1 p567 pt2 p431.
 1 tpis96 BA  1.00F   2.00     0.00     0.00     0.00 3  175.3238064    -1206000.000
   1240.000   1480.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14440.460
 0.000000000D+00 0.000000000D+00 1.515423038D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.533548254D+05-8.153942783D+01
BaF2(c)           CrI. Gurvich,1996a pt1 p567 pt2 p431.
 1 tpis96 BA  1.00F   2.00     0.00     0.00     0.00 4  175.3238064    -1206000.000
   1480.000   1641.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14440.460
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.535821388D+05-8.396607945D+01
BaF2(L)           Liquid. Gurvich,1996a pt1 p567 pt2 p431.
 1 tpis96 BA  1.00F   2.00     0.00     0.00     0.00 5  175.3238064    -1206000.000
   1641.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14440.460
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.467045237D+05-6.129240287D+01
BaH2(a)           CrII,rhombic Gurvich,1996a pt1 p556 pt2 p424.
 1 tpis96 BA  1.00H   2.00     0.00     0.00     0.00 1  139.3428800    -190000.000
    298.150    871.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9100.474
 0.000000000D+00 0.000000000D+00 4.530874339D+00 3.359308005D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.435180761D+04-1.923955725D+01
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BaH2(b)           CrI,rhombic Gurvich,1996a pt1 p556 pt2 p424.
 1 tpis96 BA  1.00H   2.00    0.00    0.00    0.00 2  139.3428800    -190000.000
    871.000   1473.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9100.474
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.589536064D+04-4.267585539D+01
BaH2(L)           Liquid Gurvich,1996a pt1 p556 pt2 p424.
 1 tpis96 BA  1.00H   2.00    0.00    0.00    0.00 3  139.3428800    -190000.000
   1473.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9100.474
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.359720958D+04-4.414413915D+01
BaI2(cr)          Rhombic. Gurvich,1996a pt1 p582 pt2 p441.
 2 tpis96 BA  1.00I   2.00    0.00    0.00    0.00 1  391.1359400    -606000.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19230.400
 1.510332529D+04-6.224807000D+02 1.545037842D+01-3.239437030D-02 9.253598890D-05
-1.251913725D-07 6.804559110D-11                -7.305629580D+04-6.364696150D+01
    500.000    984.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19230.400
-3.247335080D+02 0.000000000D+00 8.607723125D+00 2.399780624D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.555873070D+04-2.989160688D+01
BaI2(L)           Liquid. Gurvich,1996a pt1 p582 pt2 p441.
 1 tpis96 BA  1.00I   2.00    0.00    0.00    0.00 3  391.1359400    -606000.000
    984.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19230.400
 0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.611264840D+04-5.863183475D+01
BaO(cr)           Cubic Gurvich,1996a pt1 p547 pt2 p418.
 3 tpis96 BA  1.00O   1.00    0.00    0.00    0.00 1  153.3264000    -548000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
-3.734308680D+06 7.030482670D+04-5.334141930D+02 2.143135900D+00-4.664219600D-03
 5.294704440D-06-2.456512761D-09                -3.833163320D+05 2.789047565D+03
    500.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
-7.551858137D+04 0.000000000D+00 6.798957485D+00-1.205482945D-03 7.325747398D-07
 0.000000000D+00 0.000000000D+00                -6.814216420D+04-3.017618534D+01
   1400.000   2246.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
 1.380021192D+07 0.000000000D+00-1.685992319D+01 1.166250326D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.704906000D+04 1.274565988D+02
BaO(L)            Liquid Gurvich,1996a pt1 p547 pt2 p418.
 1 tpis96 BA  1.00O   1.00    0.00    0.00    0.00 3  153.3264000    -548000.000
   2246.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
 0.000000000D+00 0.000000000D+00 1.001863008D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.861430250D+04-5.267326797D+01
Ba(OH)2(b)        CrII,rhombic Gurvich,1996a pt1 p558 pt2 p427.
 1 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 1  171.3416800    -940600.000
    100.000    519.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16148.440
 5.078717800D+04-1.641996937D+03 1.964278489D+01-3.730614630D-02 1.039952734D-04
-8.659369050D-08 2.282290989D-11                -1.085585521D+05-9.701503650D+01
Ba(OH)2(a)        CrI,rhombic Gurvich,1996a pt1 p558 pt2 p427.
 1 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 2  171.3416800    -940600.000
    519.000    681.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16148.440
 0.000000000D+00 0.000000000D+00 1.491368704D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.176117467D+05-7.252241184D+01
Ba(OH)2(L)        Liquid Gurvich,1996a pt1 p558 pt2 p427.
 1 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 3  171.3416800    -940600.000
    681.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16148.440
 0.000000000D+00 0.000000000D+00 1.659749041D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.168340700D+05-8.068104197D+01
BaS(cr)           Cubic. Gurvich,1996a pt1 p584 pt2 p443.
 2 tpis96 BA  1.00S   1.00    0.00    0.00    0.00 1  169.3920000    -470000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10820.450
 3.369786470D+05-6.138740230D+03 4.922553770D+01-1.599274620D-01 3.314481350D-04
-3.600847800D-07 1.611281388D-10                -3.028248993D+04-2.539125160D+02
    500.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10820.450
-2.050631967D+04 0.000000000D+00 5.920852822D+00 8.307164223D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.839868930D+04-2.466233780D+01
BaS(L)            Liquid. Gurvich,1996a pt1 p584 pt2 p443.
 1 tpis96 BA  1.00S   1.00    0.00    0.00    0.00 3  169.3920000    -470000.000
   2500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10820.450
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.356075540D+04-3.627577743D+01
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BaSO4(a)          CrII,rhombic. Gurvich,1996a pt1 p587 pt2 p445.
 2 tpis96 BA  1.00S   1.00O   4.00     0.00     0.00 1  233.3896000   -1470000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19180.440
-1.712286968D+07 3.212789860D+05-2.441820133D+03 9.713067900D+00-2.105021811D-02
 2.383101570D-05-1.103328957D-08                  -1.624343960D+06 1.276058048D+04
    500.000   1423.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19180.440
-2.747004935D+05 0.000000000D+00 1.352094110D+01 6.200004570D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -1.820275447D+05-6.454315519D+01
BaSO4(b)          CrI,cubic. Gurvich,1996a pt1 p587 pt2 p445.
 1 tpis96 BA  1.00S   1.00O   4.00     0.00     0.00 3  233.3896000   -1470000.000
   1423.000   1853.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19180.440
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -1.842091207D+05-1.050884025D+02
BaSO4(L)          Liquid. Gurvich,1996a pt1 p587 pt2 p435.
 1 tpis96 BA  1.00S   1.00O   4.00     0.00     0.00 4  233.3896000   -1470000.000
   1853.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19180.440
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -1.793982539D+05-1.024921441D+02
Be(a)             Alpha. Ref-Elm. Alcock,1993.
 2 srd 93 BE  1.00    0.00     0.00     0.00     0.00 1    9.0121820          0.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
 3.532378938D+03 0.000000000D+00-1.827528020D+00 1.895481514D-02-2.121592253D-05
 0.000000000D+00 0.000000000D+00                  -9.832146860D+01 6.866894114D+00
    298.150   1543.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
-7.064757875D+04 0.000000000D+00 2.550360755D+00 6.848268870D-04 1.157013462D-07
 0.000000000D+00 0.000000000D+00                  -1.028803669D+03-1.399471510D+01
Be(b)             Beta. Ref-Elm. Alcock,1993.
 1 srd 93 BE  1.00    0.00     0.00     0.00     0.00 2    9.0121820          0.000
   1543.000   1563.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
 0.000000000D+00 0.000000000D+00 3.608150089D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -8.524497790D+02-2.002895768D+01
Be(L)             Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 BE  1.00    0.00     0.00     0.00     0.00 3    9.0121820          0.000
   1563.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
 0.000000000D+00 0.000000000D+00 3.545608821D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                   2.074755804D+02-1.895341257D+01
BeAL2O4(cr)       Chase,1998 pp139-41.
 3 j12/79 BE  1.00AL  2.00O   4.00     0.00     0.00 1  126.9728580   -2300782.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13088.000
 5.671733300D+05-8.864346630D+03 4.407635150D+01-3.612460380D-02 3.491655240D-05
-1.451255323D-08 0.000000000D+00                  -2.361266575D+05-2.603504873D+02
    600.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13088.000
 3.035781649D+07-2.195328809D+05 6.571002230D+02-9.751675120D-01 8.342636270D-04
-3.757959390D-07 6.972665420D-11                  9.154378130D+05-4.048262870D+03
   1200.000   2146.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13088.000
 5.346540420D+06-2.333165977D+04 6.465121650D+01-5.623102150D-02 4.944443190D-05
-2.347465372D-08 4.584679740D-12                  -1.453507980D+05-3.997587750D+02
BeAL2O4(L)        Chase,1998 pp139-41.
 1 j12/79 BE  1.00AL  2.00O   4.00     0.00     0.00 2  126.9728580   -2300782.000
   2146.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13088.000
 0.000000000D+00 0.000000000D+00 2.963602185D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -2.805665995D+05-1.711673740D+02
BeBr2(cr)         Cr,rhombic. Gurvich,1996a pt1 p376 pt2 p301.
 1 tpis96 BE  1.00BR  2.00    0.00     0.00     0.00 1  168.8201820    -358000.000
    298.150    781.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14900.000
-1.296528599D+05 0.000000000D+00 9.544519160D+00 8.967455689D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -4.637767130D+04-4.238810553D+01
BeBr2(L)          Liquid.Gurvich,1996a pt1 p376 pt2 p301.
 1 tpis96 BE  1.00BR  2.00    0.00     0.00     0.00 2  168.8201820    -358000.000
    781.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14900.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -4.571223050D+04-5.534538359D+01
BeCO3(cr)         Gurvich,1996a pt1 p385 pt2 p310.
 1 tpis96 BE  1.00C   1.00O   3.00     0.00     0.00 1   69.0210820   -1045000.000
    298.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9200.480
-3.688732108D+05 0.000000000D+00 1.057428520D+01 4.670148932D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                  -1.302813975D+05-5.746109667D+01
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BeCL2(a)          Cr,rhombic. Gurvich,1996a pt1 p370 pt2 p296.
 1 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 1   79.9181820    -496200.000
    200.000    676.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11420.000
-9.696336540D+05 1.653841300D+04-1.120322868D+02 4.343457410D-01-8.234422230D-04
 7.967601960D-07-3.089202126D-10                 -1.372167152D+05 5.981191760D+02
BeCL2(b)          CrI. Gurvich,1996a pt1 p370 pt2 p296.
 1 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 2   79.9181820    -496200.000
    676.000    688.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11420.000
 0.000000000D+00 0.000000000D+00 8.056999150D+00 2.516083329D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.169505530D+04-3.701517264D+01
BeCL2(L)          Liquid.Gurvich,1996a pt1 p370 pt2 p296.
 1 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 3   79.9181820    -496200.000
    688.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11420.000
 0.000000000D+00 0.000000000D+00 1.106499361D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.212751630D+04-5.342382325D+01
BeF2(a)           CrII,hexagonal.Gurvich,1996a pt1 p364 pt2 p292.
 1 tpis96 BE  1.00F   2.00    0.00    0.00    0.00 1   47.0089884    -1027000.000
    200.000    493.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8468.000
 3.082582728D+05-5.000745390D+03 3.049066381D+01-5.416146720D-02 5.846680620D-05
 0.000000000D+00 0.000000000D+00                 -1.011928897D+05-1.687961461D+02
BeF2(b)           CrI,hexagonal.Gurvich,1996a pt1 p364 pt2 p292.
 1 tpis96 BE  1.00F   2.00    0.00    0.00    0.00 2   47.0089884    -1027000.000
    493.000    823.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8468.000
 0.000000000D+00 0.000000000D+00 5.652527930D+00 3.986885577D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.252903029D+05-2.679700109D+01
BeF2(L)           Liquid.Gurvich,1996a pt1 p364 pt2 p292.
 1 tpis96 BE  1.00F   2.00    0.00    0.00    0.00 3   47.0089884    -1027000.000
    823.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8468.000
-1.882035141D+06 0.000000000D+00 1.234468417D+01-1.836548396D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.310986361D+05-6.898102574D+01
BeI2(cr)          Cr,rhombic. Gurvich,1996a pt1 p379 pt2 p304.
 1 tpis96 BE  1.00I   2.00    0.00    0.00    0.00 1  262.8211220    -191000.000
    298.150    763.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15200.000
-1.443741122D+05 0.000000000D+00 1.007828483D+01 3.371214900D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.647594661D+04-4.378170625D+01
BeI2(L)           Liquid.Gurvich,1996a pt1 p379 pt2 p304.
 1 tpis96 BE  1.00I   2.00    0.00    0.00    0.00 2  262.8211220    -191000.000
    763.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15200.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.551070377D+04-5.349837990D+01
BeO(a)            CrII,hexagonal. Gurvich,1996a pt1 p348 pt2 p278.
 2 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 1   25.0115820    -609400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         2837.000
 2.047701543D+05-2.981173217D+03 1.385643338D+01-1.581697711D-02 2.353849388D-05
-1.941029834D-08 6.520569610D-12                 -5.922219190D+04-8.231113660D+01
   1000.000   2373.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         2837.000
 1.024057237D+06 1.937465590D+03-2.170213872D+00 6.700940070D-03-1.829092628D-06
 2.757893870D-10-2.712743027D-14                 -8.276808970D+04 1.896607400D+01
BeO(b)            CrI,tetragonal. Gurvich,1996a pt1 p348 pt2 p278.
 1 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 2   25.0115820    -609400.000
   2373.000   2851.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         2837.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.674474850D+04-3.937528813D+01
BeO(L)            Liquid. Gurvich,1996a pt1 p348 pt2 p278.
 1 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 3   25.0115820    -609400.000
   2851.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         2837.000
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.600243170D+04-6.253805395D+01
Be(OH)2(b)        Rhombic,beta.Gurvich,1996a pt1 p359 pt2 p289.
 2 tpis96 BE  1.00O   2.00H   2.00    0.00    0.00 1   43.0268620    -905700.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8293.440
-2.821507074D+07 5.306026240D+05-4.050124700D+03 1.608285663D+01-3.491136410D-02
 3.956008990D-05-1.833019806D-08                 -2.495097922D+06 2.114570392D+04
    500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8293.440
-4.549275904D+05 0.000000000D+00 1.198362862D+01 2.034996650D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.141192354D+05-6.597431876D+01
BeS(cr)           Cr,cubic. Gurvich,1996a pt1 p381 pt2 p306.
 1 tpis96 BE  1.00S   1.00    0.00    0.00    0.00 1   41.0771820    -236000.000
    298.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5500.480
-1.061156941D+05 0.000000000D+00 4.876054031D+00 1.363880734D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.025444334D+04-2.469606404D+01
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BeSO4(a)          CrIII,tetr. Gurvich,1996a pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00     0.00     0.00 1  105.0747820   -1200000.000
    200.000    861.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12970.000
 9.674052850D+05-1.525976877D+04 9.078019340D+01-2.151323890D-01 3.405813330D-04
-2.623119799D-07 8.137303080D-11                -7.417050650D+04-5.024380540D+02
BeSO4(b)          CrII,rhombic. Gurvich,1996a pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00     0.00     0.00 2  105.0747820   -1200000.000
    861.000    912.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12970.000
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.508085273D+05-9.670719282D+01
BeSO4(c)          CrI,cubic. Gurvich,1996a pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00     0.00     0.00 3  105.0747820   -1200000.000
    912.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12970.000
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.505559568D+05-9.643025148D+01
BeSO4(L)          Liquid. Gurvich,1996a pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00     0.00     0.00 4  105.0747820   -1200000.000
   1400.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12970.000
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.498343268D+05-9.591480146D+01
Be2C(cr)          Barin,1989. Barin,1973.
 1 bar 89 BE  2.00C   1.00     0.00     0.00     0.00 1   30.0350640    -116984.640
    298.150   2400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 4.437364559D+00 2.569424296D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.550714068D+04-2.408584259D+01
Be2C(L)           Barin,1989. Barin,1973.
 1 bar 89 BE  2.00C   1.00     0.00     0.00     0.00 2   30.0350640    -116984.640
   2400.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 1.107076665D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.496946374D+04-6.577435374D+01
Be3N2(a)          CrII,cubic. Gurvich,1996a pt1 p384 pt2 p309.
 2 tpis96 BE  3.00N   2.00     0.00     0.00     0.00 1   55.0499460    -588000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7124.000
 6.443341310D+05-9.239880870D+03 4.211333200D+01-4.513325350D-02 3.232975930D-05
 0.000000000D+00 0.000000000D+00                -2.674920290D+04-2.511544265D+02
    500.000   1673.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7124.000
-2.278465381D+05 4.432191420D+02 1.376274664D+00 3.225384830D-02-2.704770612D-05
 8.116575420D-09-6.682374890D-14                -7.562743780D+04-1.197625563D+01
Be3N2(b)          CrI,hexagonal. Gurvich,1996a pt1 p384 pt2 p309.
 1 tpis96 BE  3.00N   2.00     0.00     0.00     0.00 2   55.0499460    -588000.000
   1673.000   2473.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7124.000
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.850942150D+04-1.016302777D+02
Be3N2(L)          Liquid. Gurvich,1996a pt1 p384 pt2 p309.
 1 tpis96 BE  3.00N   2.00     0.00     0.00     0.00 3   55.0499460    -588000.000
   2473.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7124.000
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.182303830D+04-1.169540588D+02
Br2(cr)           Rhombic. Gurvich,1989 pt2 p314. Chase,1998 p471 (6/82).
 1 g 8/01 BR  2.00     0.00     0.00     0.00     0.00 1  159.8080000          0.000
    200.000    265.9007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24520.000
-5.550117110D+06 1.610953162D+05-1.913542203D+03 1.201711944D+01-4.170621540D-02
 7.615296370D-05-5.694588430D-08                -6.565415920D+05 9.135571000D+03
Br2(L)            Liq.Ref-Elm.Gurvich,1989 pt2 p314.Chase,1998 p471(6/82).
 2 g 8/01 BR  2.00     0.00     0.00     0.00     0.00 2  159.8080000          0.000
    265.900    332.5037 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24520.000
 5.661619720D+06-6.002788720D+04 3.963572800D+01 2.194289283D+00-1.209616100D-02
 2.608732123D-05-2.065978604D-08                3.167204530D+05-6.832596160D+02
    332.503   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         24520.000
 0.000000000D+00 0.000000000D+00 9.056697268D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.699852754D+03-3.329354185D+01
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C(gr)             Graphite. Ref-Elm. TRC(4/83) vc,uc,tc1000-1002.
 3 n 4/83 C   1.00    0.00    0.00    0.00    0.00 1   12.0107000          0.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1053.500
 1.132856760D+05-1.980421677D+03 1.365384188D+01-4.636096440D-02 1.021333011D-04
-1.082893179D-07 4.472258860D-11                 8.943859760D+03-7.295824740D+01
    600.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1053.500
 3.356004410D+05-2.596528368D+03 6.948841910D+00-3.484836090D-03 1.844192445D-06
-5.055205960D-10 5.750639010D-14                 1.398412456D+04-4.477183040D+01
   2000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1053.500
 2.023105106D+05-1.138235908D+03 3.700279500D+00-1.833807727D-04 6.343683250D-08
-7.068589480D-12 3.335435980D-16                 5.848134850D+03-2.350925275D+01
Ca(a)             Alpha. Ref-Elm. Alcock,1993.
 2 srd 93 CA  1.00    0.00    0.00    0.00    0.00 1   40.0780000          0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5782.945
 2.209214594D+04 0.000000000D+00-2.387095323D+00 4.674833430D-02-1.481690580D-04
 1.686114356D-07 0.000000000D+00                -3.160902334D+02 9.998907900D+00
    298.150    716.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5782.945
 8.959632100D+03 0.000000000D+00 2.440591375D+00 1.722094077D-03 4.744000490D-07
 0.000000000D+00 0.000000000D+00                -7.783440840D+02-9.273708050D+00
Ca(b)             Beta. Ref-Elm. Alcock,1993.
 1 srd 93 CA  1.00    0.00    0.00    0.00    0.00 2   40.0780000          0.000
    716.000   1115.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5782.945
 0.000000000D+00 0.000000000D+00 5.701117685D+00-5.810564904D-03 4.022125176D-06
 0.000000000D+00 0.000000000D+00                -1.516788311D+03-2.607588230D+01
Ca(L)             Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 CA  1.00    0.00    0.00    0.00    0.00 3   40.0780000          0.000
   1115.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5782.945
 0.000000000D+00 0.000000000D+00 4.570323447D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.822680100D+02-2.119893317D+01
CaBr2(cr)         Rhombic Gurvich,1996a pt1 p473 pt2 p368.
 1 tpis96 CA  1.00BR  2.00    0.00    0.00    0.00 1  199.8860000    -683800.000
    298.150   1015.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17000.490
-2.826384237D+04 0.000000000D+00 8.872561342D+00 1.586623866D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.505243950D+04-3.554898721D+01
CaBr2(L)          Liquid Gurvich,1996a pt1 p473 pt2 p368.
 1 tpis96 CA  1.00BR  2.00    0.00    0.00    0.00 2  199.8860000    -683800.000
   1015.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17000.490
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.390932270D+04-5.231487518D+01
CaCO3(cr)         Hexagonal Gurvich,1996a pt1 p483 pt2 p376.
 2 tpis96 CA  1.00C   1.00O   3.00    0.00    0.00 1  100.0869000   -1206600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14480.499
-1.329862425D+07 2.500517168D+05-1.907177167D+03 7.616666270D+00-1.655870860D-02
 1.879382277D-05-8.720713270D-09                -1.271058215D+06 9.957497560D+03
    500.000   1603.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14480.499
-2.583555736D+05 0.000000000D+00 1.197256363D+01 3.263812299D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.497009803D+05-5.961133653D+01
CaCO3(L)          Liquid Gurvich,1996a pt1 p483 pt2 p376.
 1 tpis96 CA  1.00C   1.00O   3.00    0.00    0.00 3  100.0869000   -1206600.000
   1603.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14480.499
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.526719277D+05-1.052847193D+02
CaCL2(cr)         Rhombic. Gurvich,1996a pt1 p467 pt2 p365.
 2 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 1  110.9840000    -795800.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15300.460
 6.000206010D+03-4.466152170D+02 8.199988600D+00 2.374917562D-02-1.002337283D-04
 1.782027609D-07-1.141389034D-10                -9.606057780D+04-3.912159570D+01
    500.000   1048.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15300.460
-3.018818908D+04 0.000000000D+00 8.644766799D+00 1.529735366D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.845880750D+04-3.684266549D+01
CaCL2(L)          Liquid. Gurvich,1996a pt1 p467 pt2 p365.
 1 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 2  110.9840000    -795800.000
   1048.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15300.460
 2.661491778D+06 0.000000000D+00 1.078355790D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.391818610D+04-4.566953897D+01
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CaF2(a)            CrII,cubic.Gurvich,1996a pt1 p461 pt2 p361.
 3 tpis96 CA  1.00F   2.00     0.00     0.00     0.00 1   78.0748064    -1228000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11640.000
-9.875281260D+05 1.337426670D+04-6.261903110D+01 1.617894422D-01-1.271795719D-04
 0.000000000D+00 0.000000000D+00                 -2.146045473D+05 3.617287210D+02
    500.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11640.000
-6.961842180D+06 4.692065010D+04-1.157708151D+02 1.655025287D-01-1.108459197D-04
 3.213053720D-08 0.000000000D+00                 -4.101016540D+05 7.419533450D+02
   1000.000   1424.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11640.000
 1.438558077D+09 7.852955040D+05-1.342916213D+04 2.192783112D+01-1.383442475D-02
 3.122877330D-06 0.000000000D+00                  2.168972069D+06 7.823794920D+04
CaF2(b)            CrI,cubic.Gurvich,1996a pt1 p461 pt2 p361.
 1 tpis96 CA  1.00F   2.00     0.00     0.00     0.00 2   78.0748064    -1228000.000
   1424.000   1691.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11640.000
 1.535768139D+08 0.000000000D+00-1.699774473D+02 7.733123360D-02 3.585714680D-07
 0.000000000D+00 0.000000000D+00                  1.356828739D+05 1.185723820D+03
CaF2(L)            Liquid.Gurvich,1996a pt1 p461 pt2 p361.
 1 tpis96 CA  1.00F   2.00     0.00     0.00     0.00 3   78.0748064    -1228000.000
   1691.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11640.000
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.479539740D+05-5.967665213D+01
CaH2(a)            CrII,rhombic Gurvich,1996a pt1 p449 pt2 p354.
 1 tpis96 CA  1.00H   2.00     0.00     0.00     0.00 1   42.0938800     -177000.000
    298.150   1053.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6770.474
 0.000000000D+00 0.000000000D+00 3.599731073D+00 4.465566822D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.255982511D+04-1.686197756D+01
CaH2(b)            CrI,cubic Gurvich,1996a pt1 p449 pt2 p354.
 1 tpis96 CA  1.00H   2.00     0.00     0.00     0.00 2   42.0938800     -177000.000
   1053.000   1273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6770.474
 0.000000000D+00 0.000000000D+00 8.298745206D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.422633646D+04-4.409678633D+01
CaH2(L)            Liquid Gurvich,1996a pt1 p449 pt2 p354.
 1 tpis96 CA  1.00H   2.00     0.00     0.00     0.00 3   42.0938800     -177000.000
   1273.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6770.474
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.249899474D+04-4.717727797D+01
CaI2(cr)           Hexagonal Gurvich,1996a pt1 p476 pt2 p371.
 2 tpis96 CA  1.00I   2.00     0.00     0.00     0.00 1  293.8869400     -536400.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17970.499
-1.811328452D+06 3.127451814D+04-2.136599007D+02 8.328705880D-01-1.721725832D-03
 1.878967812D-06-8.440013400D-10                 -2.101977983D+05 1.142802698D+03
    500.000   1056.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17970.499
-6.638996165D+03 0.000000000D+00 8.652825001D+00 2.284560365D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.721736780D+04-3.254333551D+01
CaI2(L)            Liquid Gurvich,1996a pt1 p476 pt2 p371.
 1 tpis96 CA  1.00I   2.00     0.00     0.00     0.00 3  293.8869400     -536400.000
   1056.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17970.499
 0.000000000D+00 0.000000000D+00 1.238798197D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.485425310D+04-5.137218163D+01
CaO(cr)            Cubic Gurvich,1996a pt1 p442 pt2 p348.
 2 tpis96 CA  1.00O   1.00     0.00     0.00     0.00 1   56.0774000     -634920.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6750.499
-4.775526940D+06 9.037711420D+04-6.944320810D+02 2.802477174D+00-6.129403220D-03
 6.982167800D-06-3.247543840D-09                 -4.829411430D+05 3.619046320D+03
    500.000   3172.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6750.499
-1.459376440D+05 0.000000000D+00 7.174205094D+00-1.959947129D-03 1.291116374D-06
-2.077091735D-10 0.000000000D+00                 -7.891525080D+04-3.658562837D+01
CaO(L)             Liquid Gurvich,1996a pt1 p442 pt2 p348.
 1 tpis96 CA  1.00O   1.00     0.00     0.00     0.00 3   56.0774000     -634920.000
   3172.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6750.499
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.991857230D+04-5.908720013D+01
Ca(OH)2(cr)        Hexagonal Gurvich,1996a pt1 p454 pt2 p357.
 2 tpis96 CA  1.00O   2.00H    2.00     0.00     0.00 1   74.0926800     -985900.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14160.490
-2.058838935D+05 6.172554490D+03-7.499750990D+01 5.012182400D-01-1.423348682D-03
 1.994984415D-06-1.095038067D-09                 -1.452026205D+05 3.552445040D+02
    500.000   1023.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14160.490
-1.245413139D+05 0.000000000D+00 1.073593032D+01 3.982435525D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.223707243D+05-5.302395390D+01
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Ca(OH)2(L)          Liquid Gurvich,1996a pt1 p454 pt2 p357.
 1 tpis96 CA  1.00O   2.00H   2.00    0.00    0.00 3   74.0926800    -985900.000
   1023.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14160.490
 0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.245191822D+05-9.860760364D+01
CaS(cr)             Cubic Gurvich,1996a pt1 p478 pt2 p373.
 2 tpis96 CA  1.00S   1.00    0.00    0.00    0.00 1   72.1430000    -475000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9010.499
 4.758681130D+06-8.840702110D+04 6.675047510D+02-2.576855161D+00 5.527281760D-03
-6.202901900D-06 2.852128154D-09                3.401344700D+05-3.494344760D+03
    500.000   2800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9010.499
-1.428827435D+04 0.000000000D+00 5.567375588D+00 1.006673875D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.888163400D+04-2.530572359D+01
CaS(L)              Liquid Gurvich,1996a pt1 p478 pt2 p373.
 1 tpis96 CA  1.00S   1.00    0.00    0.00    0.00 3   72.1430000    -475000.000
   2800.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9010.499
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.348566620D+04-3.924995523D+01
CaSO4(II)           Rhombic Gurvich,1996a pt1 p481 pt2 p375.
 2 tpis96 CA  1.00S   1.00O   4.00    0.00    0.00 1  136.1406000   -1434000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17200.499
-1.361977472D+07 2.584929291D+05-1.984800641D+03 7.969448170D+00-1.736805219D-02
 1.974370111D-05-9.168768090D-09                -1.334631522D+06 1.035139350D+04
    500.000   1473.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17200.499
-2.983940124D+05 0.000000000D+00 1.359671225D+01 5.857230312D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.777846313D+05-6.802481458D+01
CaSO4(I)            Cubic Gurvich,1996a pt1 p481 pt2 p375.
 1 tpis96 CA  1.00S   1.00O   4.00    0.00    0.00 3  136.1406000   -1434000.000
   1473.000   1733.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17200.499
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.798298668D+05-1.045004358D+02
CaSO4(L)            Liquid Gurvich,1996a pt1 p481 pt2 p375.
 1 tpis96 CA  1.00S   1.00O   4.00    0.00    0.00 4  136.1406000   -1434000.000
   1733.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17200.499
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.764622601D+05-1.025572120D+02
Cd(cr)              Crystal. Ref-Elm. Cox,1989 p223.
 1 coda89 CD  1.00    0.00    0.00    0.00    0.00 1  112.4110000          0.000
    100.000    594.2587 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6247.000
 1.375273221D+05-3.221590070D+03 3.121905502D+01-1.226136798D-01 2.838880568D-04
-3.286884020D-07 1.520469817D-10                1.302807037D+04-1.551324136D+02
Cd(L)               Liquid. Ref-Elm. Cox,1989 p223.
 1 coda89 CD  1.00    0.00    0.00    0.00    0.00 2  112.4110000          0.000
    594.258   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6247.000
 0.000000000D+00 0.000000000D+00 3.596122922D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.220394750D+02-1.323298164D+01
Co(a)               Alpha. Ref-Elm. Chase,1998 pp943-6.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 1   58.9332000          0.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
-8.651834510D+05 1.462135206D+04-9.971089110D+01 3.794338600D-01-7.800106350D-04
 8.553583960D-07-3.890151670D-10                -6.795963460D+04 5.306550210D+02
    500.000    700.1007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
-9.877560740D+05 6.820602200D+03-1.521637485D+01 2.234541680D-02-9.019246600D-06
 0.000000000D+00 0.000000000D+00                -3.852839040D+04 1.014399403D+02
Co(b)               Beta.Ref-Elm.Below Lambda trans. Chase,1998 pp943-6.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 2   58.9332000          0.000
    700.100    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
 0.000000000D+00 0.000000000D+00 2.125113886D+00 2.218475342D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.197709420D+02-8.944546990D+00
    800.000   1394.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
-1.576349295D+09 9.154318170D+06-2.197967504D+04 2.793356668D+01-1.980310380D-02
 7.425124740D-06-1.149433030D-09                -5.182198410D+07 1.399846247D+05
Co(b)               Beta. Ref-Elm.Above Lambda trans. Chase,1998 pp943-6.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 3   58.9332000          0.000
   1394.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
 0.000000000D+00 0.000000000D+00 3.070872109D+02-2.155487195D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.139292950D+05-1.913104819D+03
   1400.000   1768.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
 1.648338062D+09-4.036220190D+06 3.722685700D+03-1.526326566D+00 2.354674115D-04
 0.000000000D+00 0.000000000D+00                2.649010262D+07-2.751466647D+04
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Co(L)             Liquid. Ref-Elm. Chase,1998 pp943-6.
 1 j 9/67 CO  1.00     0.00     0.00     0.00     0.00 4    58.9332000           0.000
   1768.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4771.000
 0.000000000D+00 0.000000000D+00 4.871122892D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.761381676D+02-2.448402276D+01
Cr(cr)            Below lambda trans. Ref-Elm. Chase,1998 pp959-62.
 1 j 6/73 CR  1.00     0.00     0.00     0.00     0.00 1    51.9961000           0.000
    200.000     311.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4057.000
 8.051084050D+05-1.339842819D+04 8.273507290D+01-2.075857041D-01 2.008764131D-04
 0.000000000D+00 0.000000000D+00                 6.182357950D+04-4.559971660D+02
Cr(cr)            Above lambda trans. Ref-Elm. Chase,1998 pp959-62.
 2 j 6/73 CR  1.00     0.00     0.00     0.00     0.00 2    51.9961000           0.000
    311.500    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4057.000
-2.534425357D+05 3.119404093D+03-1.358439770D+01 4.323570220D-02-5.624102820D-05
 3.652910710D-08-8.973298370D-12                -1.606559079D+04 7.858043710D+01
   1000.000    2130.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4057.000
-3.005006418D+07 1.264410306D+05-2.139399408D+02 1.937684814D-01-9.423205780D-05
 2.445139082D-08-2.606793685D-12                -7.582388710D+05 1.441907828D+03
Cr(L)             Liquid. Ref-Elm. Chase,1998 pp959-62.
 1 j 6/73 CR  1.00     0.00     0.00     0.00     0.00 3    51.9961000           0.000
   2130.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4057.000
 0.000000000D+00 0.000000000D+00 4.730284767D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.755633080D+02-2.453179007D+01
CrN(cr)           Chase,1998 p966.
 3 j12/73 CR  1.00N    1.00     0.00     0.00     0.00 1    66.0028000    -117152.000
    200.000     298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7705.000
 0.000000000D+00 0.000000000D+00-1.314063090D+00 2.565693051D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.483864491D+04 4.372952650D+00
    298.150     400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7705.000
 1.223200207D+06 0.000000000D+00-2.407090178D+01 5.583146740D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.292218790D+03 1.319158541D+02
    400.000    2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7705.000
-2.661907798D+05 1.615547039D+03 1.892576742D+00 4.987173370D-03-2.514705667D-06
 7.617792270D-10-9.124276740D-14                -2.496407842D+04-3.735659490D+00
Cr2N(cr)          JPCRD 1998 Mono.9 p971.
 3 j12/73 CR  2.00N    1.00     0.00     0.00     0.00 1   117.9989000    -125520.000
    298.150     700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 5.676714650D+06-6.561919460D+04 2.971622148D+02-6.132148300D-01 6.373067250D-04
-2.569754132D-07 0.000000000D+00                 3.113488256D+05-1.716694497D+03
    700.000    1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 8.246680410D+05-1.965549089D+03 5.659967790D+00 1.366241998D-02-1.241835551D-05
 6.313550760D-09-1.192405400D-12                -3.594772610D+03-3.071970867D+01
   1500.000    2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 4.325258320D+09-1.355254539D+07 1.757503878D+04-1.205560629D+01 4.623646210D-03
-9.389890050D-07 7.891119490D-11                 8.506076540D+07-1.227417790D+05
Cr2O3(I')         Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.
 1 tpis82 CR  2.00O    3.00     0.00     0.00     0.00 1   151.9904000   -1140600.000
    200.000     306.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15300.000
-2.112979833D+06 0.000000000D+00 2.207431906D+02-1.164973854D+00 1.853971249D-03
 0.000000000D+00 0.000000000D+00                -1.746831159D+05-9.949025210D+02
Cr2O3(I)          Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.
 1 tpis82 CR  2.00O    3.00     0.00     0.00     0.00 2   151.9904000   -1140600.000
    306.000     310.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15300.000
 0.000000000D+00 0.000000000D+00 6.705915562D+03-4.303760534D+01 6.919229155D-02
 0.000000000D+00 0.000000000D+00                -8.349875160D+05-2.844167579D+04
Cr2O3(I)          Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.
 1 tpis82 CR  2.00O    3.00     0.00     0.00     0.00 3   151.9904000   -1140600.000
    310.000     335.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15300.000
 0.000000000D+00 0.000000000D+00 2.443570337D+02-1.399445548D+00 2.113509996D-03
 0.000000000D+00 0.000000000D+00                -1.665032895D+05-1.059172219D+03
Cr2O3(I)          Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.
 1 tpis82 CR  2.00O    3.00     0.00     0.00     0.00 4   151.9904000   -1140600.000
    335.000    2705.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15300.000
-3.415474875D+05 0.000000000D+00 1.616932327D+01-1.517828471D-03 1.014852348D-06
 0.000000000D+00 0.000000000D+00                -1.430478214D+05-8.374919535D+01
Cr2O3(L)          Liquid. Gurvich,1982 pt1 p18 pt2 p22.
 1 tpis82 CR  2.00O    3.00     0.00     0.00     0.00 5   151.9904000   -1140600.000
   2705.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15300.000
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.383139935D+05-1.123603099D+02
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Cs(cr)              Crystal. Ref-Elm. Cox,1989 p263.
 1 coda89 CS  1.00     0.00     0.00     0.00     0.00 1  132.9054500           0.000
    100.000    301.5907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7711.000
 6.519841350D+04-1.756639077D+03 1.999681093D+01-6.938328820D-02 1.093682552D-04
 0.000000000D+00 0.000000000D+00                 6.382890840D+03-9.338251570D+01
Cs(L)               Liquid. Ref-Elm. Cox,1989 p263.
 2 coda89 CS  1.00     0.00     0.00     0.00     0.00 2  132.9054500           0.000
    301.590   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7711.000
-4.218078030D+04-1.745861711D+01 5.702246950D+00-5.113948550D-03 3.201752440D-06
-1.767959558D-10 4.827862700D-14                -1.290810964D+03-2.031478114D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7711.000
-7.255372990D+05 3.001930225D+03 1.782289032D-01 2.832281079D-04 1.810515176D-07
 7.718855550D-10-8.889289510D-14                -1.920877274D+04 1.635273378D+01
CsBO2(cr)           Cubic. Gurvich,1982 pt1 p504 pt2 p525.
 2 tpis82 CS  1.00B    1.00O    2.00     0.00     0.00 1  175.7152500    -962000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14368.000
 1.241529552D+07-2.256720327D+05 1.662515290D+03-6.320716230D+00 1.337407484D-02
-1.484168930D-05 6.761667750D-09                 9.049643320D+05-8.739017110D+03
    500.000   1005.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14368.000
-1.344267330D+05 0.000000000D+00 1.014162565D+01 3.564309650D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.193344436D+05-4.705131010D+01
CsBO2(L)            Liquid. Gurvich,1982 pt1 p504 pt2 p525.
 1 tpis82 CS  1.00B    1.00O    2.00     0.00     0.00 2  175.7152500    -962000.000
   1005.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14368.000
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.214875849D+05-9.061903610D+01
CsBr(cr)            Cubic. Gurvich,1982 pt1 p488 pt2 p511.
 2 tpis82 CS  1.00BR   1.00     0.00     0.00     0.00 1  212.8094500    -405600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13135.000
 8.214717410D+05-1.533809444D+04 1.213999610D+02-4.502622350D-01 9.722874060D-04
-1.094185412D-06 5.042592550D-10                 1.851486523D+04-6.252270680D+02
    500.000    910.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13135.000
 0.000000000D+00 0.000000000D+00 5.882254010D+00 1.622332026D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.060809300D+04-2.041491096D+01
CsBr(L)             Liquid. Gurvich,1982 pt1 p488 pt2 p511.
 1 tpis82 CS  1.00BR   1.00     0.00     0.00     0.00 2  212.8094500    -405600.000
    910.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13135.000
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.995364530D+04-3.720087044D+01
CsCL(a)             Cubic. Gurvich,1982 pt1 p485 pt2 p508.
 2 tpis82 CS  1.00CL   1.00     0.00     0.00     0.00 1  168.3584500    -442310.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12450.000
-1.703772998D+06 3.247452440D+04-2.455466631D+02 1.009178034D+00-2.207551915D-03
 2.517334138D-06-1.172381667D-09                -2.005014179D+05 1.287839193D+03
    500.000    743.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12450.000
-3.937950690D+04 0.000000000D+00 6.626999920D+00 4.235262420D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.532407590D+04-2.593783387D+01
CsCL(b)             Cubic. Gurvich,1982 pt1 p485 pt2 p508.
 1 tpis82 CS  1.00CL   1.00     0.00     0.00     0.00 2  168.3584500    -442310.000
    743.000    919.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12450.000
 0.000000000D+00 0.000000000D+00 7.841712861D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.570430740D+04-3.314329722D+01
CsCL(L)             Liquid. Gurvich,1982 pt1 p485 pt2 p508.
 1 tpis82 CS  1.00CL   1.00     0.00     0.00     0.00 3  168.3584500    -442310.000
    919.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12450.000
 0.000000000D+00 0.000000000D+00 8.839967719D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.417056700D+04-3.728749769D+01
CsF(cr)             Cubic. Gurvich,1982 pt1 p481 pt2 p505.
 2 tpis82 CS  1.00F    1.00     0.00     0.00     0.00 1  151.9038532    -557100.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11760.000
-2.453746682D+06 4.440981600D+04-3.216355300D+02 1.258524529D+00-2.661147803D-03
 2.959315715D-06-1.350383298D-09                -2.700040022D+05 1.698453355D+03
    500.000    976.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11760.000
 0.000000000D+00 0.000000000D+00 5.088206230D+00 3.543462080D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.867788740D+04-1.886662026D+01
CsF(L)              Liquid. Gurvich,1982 pt1 p481 pt2 p505.
 1 tpis82 CS  1.00F    1.00     0.00     0.00     0.00 2  151.9038532    -557100.000
    976.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11760.000
 0.000000000D+00 0.000000000D+00 8.659560215D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.786592520D+04-3.731740982D+01
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CsH(cr)            Cubic. Gurvich,1982 pt1 p476 pt2 p500.
 1 tpis82 CS  1.00H   1.00     0.00     0.00     0.00 1  133.9133900     -54040.000
    298.150    801.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10500.000
-5.041788392D+04 0.000000000D+00 4.142517118D+00 4.385946977D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -8.098615840D+03-1.641381626D+01
CsH(L)             Liquid. Gurvich,1982 pt1 p476 pt2 p500.
 1 tpis82 CS  1.00H   1.00     0.00     0.00     0.00 2  133.9133900     -54040.000
    801.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10500.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.901332940D+03-2.794351109D+01
CsI(cr)            Cubic. Gurvich,1982 pt1 p492 pt2 p514.
 2 tpis82 CS  1.00I   1.00     0.00     0.00     0.00 1  259.8099200     -348100.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13470.000
 1.754014150D+06-3.232916500D+04 2.467159187D+02-9.287377130D-01 1.973235969D-03
-2.193580686D-06 1.003390730D-09                 1.023639971D+05-1.282961001D+03
    500.000    905.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13470.000
-1.690343843D+04 0.000000000D+00 7.346625000D+00-4.804073480D-03 6.604565720D-06
 0.000000000D+00 0.000000000D+00                 -4.395851780D+04-2.611726446D+01
CsI(L)             Liquid. Gurvich,1982 pt1 p492 pt2 p514.
 1 tpis82 CS  1.00I   1.00     0.00     0.00     0.00 2  259.8099200     -348100.000
    905.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13470.000
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.226975350D+04-3.246075054D+01
CsNO2(I)           Cubic. Gurvich,1982 pt1 p498 pt2 p519.
 1 tpis82 CS  1.00N   1.00O    2.00     0.00     0.00 1  178.9109500     -379900.000
    298.150    679.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23420.000
 0.000000000D+00 0.000000000D+00 1.151300558D+01-3.537430348D-03 5.931437932D-06
 0.000000000D+00 0.000000000D+00                 -4.901898420D+04-4.387814029D+01
CsNO2(L)           Liquid. Gurvich,1982 pt1 p498 pt2 p519.
 1 tpis82 CS  1.00N   1.00O    2.00     0.00     0.00 2  178.9109500     -379900.000
    679.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23420.000
 0.000000000D+00 0.000000000D+00 1.274879698D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.874363630D+04-5.104014160D+01
CsNO3(a)           Hexagonal. Gurvich,1982 pt1 p500 pt2 p521.
 1 tpis82 CS  1.00N   1.00O    3.00     0.00     0.00 1  194.9103500     -505000.000
    200.000    427.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20050.000
-3.246405120D+06 5.377946540D+04-3.399293910D+02 1.103526542D+00-1.665374892D-03
 1.005891643D-06 0.000000000D+00                 -3.130119262D+05 1.853516509D+03
CsNO3(b)           Cubic. Gurvich,1982 pt1 p500 pt2 p521.
 1 tpis82 CS  1.00N   1.00O    3.00     0.00     0.00 2  194.9103500     -505000.000
    427.000    682.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20050.000
-8.675315803D+05 0.000000000D+00 2.211459244D+01-4.596061584D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.970758310D+04-1.102656798D+02
CsNO3(L)           Cubic. Gurvich,1982 pt1 p500 pt2 p521.
 1 tpis82 CS  1.00N   1.00O    3.00     0.00     0.00 3  194.9103500     -505000.000
    682.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20050.000
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.506630270D+04-8.345202339D+01
CsOH(b)            Beta.  Gurvich,1997.
 2 g 8/97 CS  1.00O   1.00H    1.00     0.00     0.00 1  149.9127900     -416200.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14103.000
-1.070491244D+06 2.726790967D+04-2.447999195D+02 9.717566950D-01-1.304183626D-03
 0.000000000D+00 0.000000000D+00                 -1.676915176D+05 1.260979156D+03
    298.150    498.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14103.000
 2.988510447D+05 0.000000000D+00-5.599488124D+00 4.758933479D-02-3.982976748D-05
 0.000000000D+00 0.000000000D+00                 -4.914854260D+04 3.370083195D+01
CsOH(c)            Gamma. Gurvich,1997.
 1 g 8/97 CS  1.00O   1.00H    1.00     0.00     0.00 3  149.9127900     -416200.000
    498.200    615.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14103.000
 0.000000000D+00 0.000000000D+00 8.743750383D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.198053970D+04-3.591737929D+01
CsOH(L)            Liquid. Gurvich,1997.
 1 g 8/97 CS  1.00O   1.00H    1.00     0.00     0.00 4  149.9127900     -416200.000
    615.500   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14103.000
 0.000000000D+00 0.000000000D+00 1.022309192D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.195536080D+04-4.389810453D+01
CsO2(a)            Tetragonal. Gurvich,1982 pt1 p472 pt2 p494.
 1 tpis82 CS  1.00O   2.00     0.00     0.00     0.00 1  164.9042500     -286100.000
    298.150    403.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18000.000
 0.000000000D+00 0.000000000D+00 6.423469330D+00 1.032375931D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.678373920D+04-2.259778952D+01
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Cs02(c)           Cubic. Gurvich,1982 pt1 p472 pt2 p494.
 1 tpis82 CS  1.00O   2.00     0.00     0.00     0.00 2  164.9042500    -286100.000
    403.000    723.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18000.000
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.762205990D+04-4.339551574D+01
Cs02(L)           Liquid. Gurvich,1982 pt1 p472 pt2 p494.
 1 tpis82 CS  1.00O   2.00     0.00     0.00     0.00 3  164.9042500    -286100.000
    723.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18000.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.645253810D+04-4.983623140D+01
Cs2C03(cr)        Gurvich,1982 pt1 p502 pt2 p523.
 2 tpis82 CS  2.00C   1.00O   3.00     0.00     0.00 1  325.8198000   -1134900.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25727.000
-2.861109977D+06 6.041289230D+04-5.002404530D+02 2.198717904D+00-5.002265900D-03
 5.885981300D-06-2.807201102D-09                -4.049923380D+05 2.581625553D+03
    500.000   1066.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25727.000
-2.194678436D+05 0.000000000D+00 1.478581229D+01 8.646042770D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.420250493D+05-6.346394980D+01
Cs2C03(L)         Liquid. Gurvich,1982 pt1 502 pt2 p523.
 1 tpis82 CS  2.00C   1.00O   3.00     0.00     0.00 2  325.8198000   -1134900.000
   1066.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25727.000
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.436995486D+05-1.194626528D+02
Cs2O(cr)          Hexagonal. Gurvich,1982 pt1 p472 pt2 p495.
 2 tpis82 CS  2.00O   1.00     0.00     0.00     0.00 1  281.8103000    -346400.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17680.000
-5.627068090D+05 9.379197410D+03-5.661406600D+01 2.388479040D-01-4.761089540D-04
 5.101511920D-07-2.256975084D-10                -8.742010290D+04 3.144128417D+02
    500.000    768.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17680.000
 0.000000000D+00 0.000000000D+00 7.940814720D+00 4.024410190D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.420852680D+04-2.877552024D+01
Cs2O(L)           Liquid. Gurvich,1982 pt1 p472 pt2 p495.
 1 tpis82 CS  2.00O   1.00     0.00     0.00     0.00 2  281.8103000    -346400.000
    768.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17680.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.375456510D+04-4.970156357D+01
Cs2O2(cr)         Rhombic Gurvich,1982 pt1 p475 pt2 p498.
 1 tpis82 CS  2.00O   2.00     0.00     0.00     0.00 1  297.8097000    -440000.000
    298.150    867.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21300.000
 0.000000000D+00 0.000000000D+00 1.003895599D+01 4.651506824D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.611939360D+04-3.693586892D+01
Cs2O2(L)          Liquid. Gurvich,1982 pt1 p475 pt2 p498.
 1 tpis82 CS  2.00O   2.00     0.00     0.00     0.00 2  297.8097000    -440000.000
    867.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21300.000
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.699432080D+04-7.096530706D+01
Cs2SO4(a)         Rhombohedral. Gurvich,1982 pt1 p496 pt2 p517.
 2 tpis82 CS  2.00S   1.00O   4.00     0.00     0.00 1  361.8735000   -1442900.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27740.000
-9.607719290D+06 1.823999086D+05-1.398882747D+03 5.671901780D+00-1.240281336D-02
 1.414114808D-05-6.571017390D-09                -9.952928170D+05 7.301725680D+03
    500.000    920.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27740.000
-2.673923999D+05 0.000000000D+00 1.731761674D+01 9.163180750D-03-1.678705593D-05
 2.444634119D-08 0.000000000D+00                -1.799058942D+05-7.688396220D+01
Cs2SO4(b)         Gurvich,1982 pt1 p496 pt2 p517.
 1 tpis82 CS  2.00S   1.00O   4.00     0.00     0.00 2  361.8735000   -1442900.000
    920.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27740.000
 0.000000000D+00 0.000000000D+00-2.345297558D+01 5.324523033D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.607408251D+05 1.601933430D+02
Cs2SO4(c)         Hexagonal. Gurvich,1982 pt1 p496 pt2 p517.
 1 tpis82 CS  2.00S   1.00O   4.00     0.00     0.00 3  361.8735000   -1442900.000
   1000.000   1288.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27740.000
 0.000000000D+00 0.000000000D+00 1.021611616D+01 1.412157782D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.748480906D+05-3.326085070D+01
Cs2SO4(L)         Liquid. Gurvich,1982 pt1 p496 pt2 p517.
 1 tpis82 CS  2.00S   1.00O   4.00     0.00     0.00 4  361.8735000   -1442900.000
   1288.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         27740.000
 0.000000000D+00 0.000000000D+00 2.489623562D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.778210954D+05-1.169167420D+02
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Cu(cr)              Cubic. Ref-Elm.Cox,1989 p226.
 1 coda89 CU  1.00     0.00     0.00     0.00     0.00 1   63.5460000          0.000
    200.000   1358.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5004.000
-2.455775109D+04 1.648069205D+02 2.080947143D+00 2.639078305D-03-2.714101362D-06
 1.402864982D-09-9.724321640D-14                 -1.737850969D+03-8.133166800D+00
Cu(L)               Liquid. Ref-Elm.Cox,1989 p226.
 1 coda89 CU  1.00     0.00     0.00     0.00     0.00 2   63.5460000          0.000
   1358.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5004.000
 0.000000000D+00 0.000000000D+00 3.944910764D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.111013775D+02-1.836065775D+01
CuBr(a)             Alpha. Pankratz,1984 p177.
 1 g10/00 CU  1.00BR  1.00     0.00     0.00     0.00 1  143.4500000     -105604.160
    298.150    657.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 9.282973940D+07-1.403844530D+06 8.783223470D+03-2.905323712D+01 5.373393350D-02
-5.266133060D-05 2.137926033D-08                  6.589039380D+06-4.752115490D+04
CuBr(b)             Beta. Pankratz,1984 p177.
 1 g10/00 CU  1.00BR  1.00     0.00     0.00     0.00 2  143.4500000     -105604.160
    657.000    741.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 2.030134717D+04 0.000000000D+00 8.680899310D+00 1.192698187D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.494845171D+04-3.784920540D+01
CuBr(c)             Gamma. Pankratz,1984 p177.
 1 g10/00 CU  1.00BR  1.00     0.00     0.00     0.00 3  143.4500000     -105604.160
    741.000    759.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 6.996549990D+00-2.480878428D-06 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.343768009D+04-2.630094995D+01
CuBr(L)             Liquid. Pankratz,1984 p177.
 1 g10/00 CU  1.00BR  1.00     0.00     0.00     0.00 4  143.4500000     -105604.160
    759.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 5.249558100D+06-2.757081290D+04 7.103036660D+01-7.368389880D-02 4.263508020D-05
-1.219118967D-08 1.489531692D-12                  1.442863364D+05-4.366365590D+02
CuBr2(cr)           Crystal. Pankratz,1984 p181.
 1 g10/00 CU  1.00BR  2.00     0.00     0.00     0.00 1  223.3540000     -138490.400
    298.150    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-2.314796663D+04 0.000000000D+00 9.183704151D+00 6.239886656D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.949996594D+04-3.714221219D+01
CuCL(a)             Alpha. Pankratz,1984 p182.
 1 g10/00 CU  1.00CL  1.00     0.00     0.00     0.00 1   98.9990000     -155644.800
    298.150    685.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-3.658126050D+07 4.622460750D+05-2.297616527D+03 5.656465110D+00-6.837763380D-03
 3.261042890D-06 0.000000000D+00                 -2.287516266D+06 1.303469843D+04
CuCL(b)             Beta. Pankratz,1984 p182.
 1 g10/00 CU  1.00CL  1.00     0.00     0.00     0.00 2   98.9990000     -155644.800
    685.000    696.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 9.573589740D+00-1.820889604D-05 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.177033413D+04-4.503412690D+01
CuCL(L)             Liquid. Pankratz,1984 p182.
 1 g10/00 CU  1.00CL  1.00     0.00     0.00     0.00 3   98.9990000     -155644.800
    696.000   1700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 2.136369978D+07-1.123842012D+05 2.576303311D+02-2.967521373D-01 1.937139129D-04
-6.602332990D-08 9.216872010D-12                  6.263960470D+05-1.640361694D+03
CuCL2(cr)           Crystal. Pankratz,1984 p185.
 1 g10/00 CU  1.00CL  2.00     0.00     0.00     0.00 1  134.4520000     -217986.400
    298.150    675.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-2.119456576D+04-7.996037250D+02 1.293400534D+01-6.531311580D-03 7.387791880D-06
-2.975231314D-09 0.000000000D+00                 -2.535822405D+04-6.185052500D+01
CuCL2(L)            Liquid. Pankratz,1984 p185.
 1 g10/00 CU  1.00CL  2.00     0.00     0.00     0.00 2  134.4520000     -217986.400
    675.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 9.913368316D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.929700009D+04-4.386870689D+01
CuF(cr)             Crystal. Pankratz,1984 p186.
 1 g10/00 CU  1.00F   1.00     0.00     0.00     0.00 1   82.5444032     -209200.000
    298.150   1300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 8.970191630D+04-8.507461080D+02 7.497889560D+00 2.741560003D-03-2.987072214D-06
 1.372974641D-09-2.449154828D-13                 -2.234632002D+04-3.796523780D+01
CuF2(cr)            Crystal. Pankratz,1984 p188.
 1 g10/00 CU  1.00F   2.00     0.00     0.00     0.00 1  101.5428064     -539819.680
    298.150   1109.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 2.173703718D+04-4.937180300D+02 7.140314880D+00 9.517087050D-03-7.459164380D-06
 1.904472482D-09 4.473847180D-13                 -6.452906470D+04-3.535501070D+01
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CuF2(L)            Liquid. Pankratz,1984 p188.
 1 g10/00 CU  1.00F   2.00    0.00    0.00    0.00 2  101.5428064     -539819.680
   1109.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 1.207719998D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.351133500D+04-5.654007188D+01
CuI(a)             King,1973. Pankratz,1984 p190.
 1 g11/00 CU  1.00I   1.00    0.00    0.00    0.00 1  190.4504700      -67780.800
    200.000    642.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12179.624
 3.341893600D+07-6.258598240D+05 4.752824990D+03-1.866377479D+01 4.013741700D-02
-4.477073620D-05 2.026229192D-08                 2.806623546D+06-2.484310642D+04
CuI(b)             Beta. Pankratz,1984 p190.
 1 g11/00 CU  1.00I   1.00    0.00    0.00    0.00 2  190.4504700      -67780.800
    642.000    680.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12179.624
 0.000000000D+00 0.000000000D+00 1.665647164D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.582086031D+04-8.975455543D+01
CuI(c)             Gamma. Pankratz,1984 p190.
 1 g11/00 CU  1.00I   1.00    0.00    0.00    0.00 3  190.4504700      -67780.800
    680.000    868.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12179.624
 0.000000000D+00 0.000000000D+00 8.252753319D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.787795700D+03-3.447628919D+01
CuI(L)             Liquid. Pankratz,1984 p190.
 1 g11/00 CU  1.00I   1.00    0.00    0.00    0.00 4  190.4504700      -67780.800
    868.000   1600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12179.624
-1.011252768D+08 4.982205420D+05-1.002812164D+03 1.087833779D+00-6.564648130D-04
 2.096109501D-07-2.761239948D-11                 -2.912510925D+06 6.575842050D+03
CuO(cr)            Crystal. King,1973 p56.
 2 g11/00 CU  1.00O   1.00    0.00    0.00    0.00 1   79.5454000     -155644.800
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7100.248
-4.516917320D+05 5.470078090D+03-2.199474390D+01 5.929815860D-02-4.346152590D-05
 0.000000000D+00 0.000000000D+00                -4.709485370D+04 1.305030297D+02
    500.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7100.248
 1.200465628D+06-7.265787600D+03 2.078520457D+01-1.455522591D-02 1.267438982D-05
-1.010207859D-08 3.818025500D-12                 2.099455971D+04-1.272540351D+02
Cu(OH)2(cr)        Crystal. King,1973 p62.
 1 g10/00 CU  1.00O   2.00H   2.00    0.00    0.00 1   97.5606800     -443085.600
    298.150   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-2.719377798D+05 2.064524617D+03 2.639692948D+00 1.680803576D-02-1.185312108D-05
 4.128854220D-09-5.731701790D-13                 -6.740281360D+04-3.697949500D+00
CuS(cr)            Crystal. Pankratz,1987 p99.
 1 g10/00 CU  1.00S   1.00    0.00    0.00    0.00 1   95.6110000      -55647.200
    298.150    717.8247 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-2.883682516D+06 3.709375520D+04-1.908896435D+02 5.441914820D-01-8.255987560D-04
 6.585650750D-07-2.151268669D-10                 -1.888895944D+05 1.072934856D+03
CuSO4(cr)          Crystal. King,1973 p68.
 2 g10/00 CU  1.00S   1.00O   4.00    0.00    0.00 1  159.6086000     -768600.800
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16869.888
-6.059594400D+06 1.149925970D+05-8.865821710D+02 3.621436210D+00-7.953212370D-03
 9.136099910D-06-4.293593660D-09                 -6.103352510D+05 4.617693800D+03
    500.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16869.888
 4.517267510D+06-3.693547470D+04 1.240090231D+02-1.574474634D-01 1.231374136D-04
-4.209750670D-08 3.791447690D-12                 1.020928632D+05-7.502604750D+02
Cu2O(cr)           Crystal. King,1973 p60.
 2 g10/00 CU  2.00O   1.00    0.00    0.00    0.00 1  143.0914000     -170707.200
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12598.024
 6.943093940D+05-1.107206812D+04 7.007600820D+01-1.693010736D-01 2.296941394D-04
-1.193708373D-07 0.000000000D+00                 2.971995795D+04-3.800603570D+02
    600.000   1516.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12598.024
 4.899293250D+06-3.226767710D+04 9.242913240D+01-1.133053506D-01 8.886458460D-05
-3.911779590D-08 8.170753140D-12                 1.562364374D+05-5.668285450D+02
Cu2O(L)            Liquid. King,1973 p60.
 1 g10/00 CU  2.00O   1.00    0.00    0.00    0.00 2  143.0914000     -170707.200
   1516.700   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12598.024
 0.000000000D+00 0.000000000D+00 1.199819496D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.922442298D+04-5.674847630D+01
Cu2S(a)            Alpha. Pankratz,1987 p101.
 1 g10/00 CU  2.00S   1.00    0.00    0.00    0.00 1  159.1570000      -75730.400
    298.150    376.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 1.219944245D+05 0.000000000D+00 2.442685885D+00 1.822933284D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.023757104D+04-4.696533160D+00
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Cu2S(b)           Beta. Pankratz,1987 p101.
 1 g10/00 CU  2.00S   1.00    0.00    0.00    0.00 2  159.1570000     -75730.400
    376.000    720.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-1.211638496D+06 1.256233530D+04-3.683304810D+01 9.547244050D-02-9.864227170D-05
 3.946755750D-08 0.000000000D+00                 -7.698051300D+04 2.352740334D+02
Cu2S(c)           Gamma. Pankratz,1987 p101.
 1 g10/00 CU  2.00S   1.00    0.00    0.00    0.00 3  159.1570000     -75730.400
    720.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 1.585983458D+07-9.420242290D+04 2.398981626D+02-2.943865388D-01 2.084368440D-04
-7.757369510D-08 1.184191791D-11                 5.203074640D+05-1.502163502D+03
Cu2S(L)           Liquid. Pankratz,1987 p101.
 1 g10/00 CU  2.00S   1.00    0.00    0.00    0.00 4  159.1570000     -75730.400
   1400.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.078393315D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.075259326D+04-4.551698813D+01
Fe(a)             Alpha. Ref-Elm.Below Lambda trans. Chase,1998 p1221.
 3 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 1   55.8450000         0.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 1.350490931D+04-7.803806250D+02 9.440171470D+00-2.521767704D-02 5.350170510D-05
-5.099094730D-08 1.993862728D-11                 2.416521408D+03-4.749002850D+01
    500.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 3.543032740D+06-2.447150531D+04 6.561020930D+01-7.043929680D-02 3.181052870D-05
 0.000000000D+00 0.000000000D+00                 1.345059978D+05-4.133788690D+02
    800.000   1042.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 2.661026334D+09-7.846827970D+06-7.289212280D+02 2.613888297D+01-3.494742140D-02
 1.763752622D-05-2.907723254D-09                 5.234868470D+07-1.529052200D+04
Fe(a)             Alpha. Ref-Elm.Above Lambda trans. Chase,1998 pp1221-5.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 2   55.8450000         0.000
   1042.000   1184.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 2.481923052D+08 0.000000000D+00-5.594349090D+02 3.271704940D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 6.467503430D+05 3.669168720D+03
Fe(c)             Gamma. Ref-Elm. Chase,1998 pp1221-5.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 3   55.8450000         0.000
   1184.000   1665.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 1.442428576D+09-5.335491340D+06 8.052828000D+03-6.303089630D+00 2.677273007D-03
-5.750045530D-07 4.718611960D-11                 3.264264250D+07-5.508852170D+04
Fe(d)             Delta. Ref-Elm. Chase,1998 pp1221-5.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 4   55.8450000         0.000
   1665.000   1809.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
-3.450190030D+08 0.000000000D+00 7.057501520D+02-5.442977890D-01 1.190040139D-04
 0.000000000D+00 0.000000000D+00                 -8.045725750D+05-4.545180320D+03
Fe(L)             Liquid. Ref-Elm. Chase,1998 pp1221-5.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 5   55.8450000         0.000
   1809.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 0.000000000D+00 0.000000000D+00 5.535383324D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.270608703D+03-2.948115042D+01
Fe(CO)5(L)        Liquid. Chase,1998 p697.
 1 j 3/78 FE  1.00C   5.00O   5.00    0.00    0.00 1  195.8955000    -766090.400
    253.100   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        52934.000
 0.000000000D+00 0.000000000D+00 2.811771229D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.005222674D+05-1.196624513D+02
FeCL2(cr)         Crystal. Chase,1998 pp819-21.
 1 j12/70 FE  1.00CL  2.00    0.00    0.00    0.00 1  126.7510000    -341833.000
    200.000    950.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16273.000
-3.757527240D+04 5.932070220D+00 8.822760280D+00 3.742344220D-03-4.622462850D-06
 4.041497880D-09-1.447289303D-12                 -4.403595790D+04-3.721747350D+01
FeCL2(L)          Liquid. Chase,1998 pp819-21.
 1 j12/70 FE  1.00CL  2.00    0.00    0.00    0.00 2  126.7510000    -341833.000
    950.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16273.000
 0.000000000D+00 0.000000000D+00 1.228851730D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.110842530D+04-5.319067642D+01
FeCL3(cr)         Pankratz,1984 p228. Stuve,1980.
 2 g12/00 FE  1.00CL  3.00    0.00    0.00    0.00 1  162.2040000    -399237.280
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19440.538
-4.411357940D+06 9.339652130D+04-7.909985950D+02 3.467913380D+00-7.632263650D-03
 7.316486370D-06-1.314023921D-09                 -4.596567330D+05 4.056239320D+03
    298.150    577.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19440.538
-1.373170458D+05 1.246888186D+03 4.499842520D+00 1.632234838D-02-3.871665510D-06
 0.000000000D+00 0.000000000D+00                 -5.761466240D+04-9.144353090D+00
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FeCL3(L)            Pankratz,1984 p228. Stuve,1980.
 1 g12/00 FE  1.00CL  3.00    0.00    0.00    0.00 2  162.2040000    -399237.280
    577.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19440.538
 0.000000000D+00 0.000000000D+00 1.610293331D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.849183540D+04-6.711333581D+01
Fe.947O(cr)         Wustite. Pankratz,1983 p155.
 1 g11/00 FE  0.95O   1.00    0.00    0.00    0.00 1   69.0521500    -266269.760
    298.150   1652.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-1.179193966D+04 1.388393372D+02 2.999841854D+00 1.274527210D-02-1.883886065D-05
 1.274258345D-08-3.042206479D-12                -3.417350500D+04-1.284759120D+01
Fe.947O(L)          Wustite Liquid. Pankratz,1983 p155.
 1 g11/00 FE  0.95O   1.00    0.00    0.00    0.00 2   69.0521500    -266269.760
   1652.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 8.147077819D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.255080650D+04-3.995344357D+01
FeOCL(cr)           Stuve,1980.
 2 g12/00 FE  1.00O   1.00CL  1.00    0.00    0.00 1  107.2974000    -410994.320
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12940.275
 7.211593840D+08-1.800235674D+07 1.865368524D+05-1.026861036D+03 3.167682830D+00
-5.191522260D-03 3.531434870D-06                7.557107690D+07-9.148719350D+05
    298.150    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12940.275
-2.937711808D+05 2.628264415D+03-4.552872200D+00 3.806463330D-02-5.536092880D-05
 4.502460810D-08-1.258510270D-11                -6.531943100D+04 3.377057910D+01
Fe(OH)2(cr)         Crystal. Chase,1998 p1229.
 2 j 6/66 FE  1.00O   2.00H   2.00    0.00    0.00 1   89.8596800    -574045.000
    298.150    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 4.240926040D+05-5.246013500D+03 3.564078140D+01-5.777285350D-02 8.334162550D-05
-5.353404280D-08 1.183994084D-11                -4.642385900D+04-1.937387923D+02
    800.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 8.260012740D+06-3.584848620D+04 6.631482130D+01-2.947893247D-02 4.572669670D-06
 1.317544528D-09-2.977356578D-13                1.429652898D+05-4.364616280D+02
Fe(OH)3(cr)         Crystal. Chase,1998 p1231.
 1 j 6/66 FE  1.00O   3.00H   3.00    0.00    0.00 1  106.8670200    -832616.000
    298.150   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-7.418284690D+04 4.915361510D+01 6.351612700D+00 2.730299149D-02-2.006100982D-05
 7.511526410D-09-1.262038044D-12                -1.036132609D+05-3.117351481D+01
FeS(a)              Alpha. Pankratz,1987. Chase,1998 pp1241-3 9/77.
 1 g11/00 FE  1.00S   1.00    0.00    0.00    0.00 1   87.9100000     -99621.040
    200.000    411.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9414.000
 6.562987140D+06-1.108882861D+05 7.200477640D+02-2.169002385D+00 3.009472055D-03
-1.385164934D-06 0.000000000D+00                4.996994470D+05-3.905129920D+03
FeS(b)              Beta. Pankratz,1987. Chase,1998 pp1241-3 9/77.
 1 g11/00 FE  1.00S   1.00    0.00    0.00    0.00 2   87.9100000     -99621.040
    411.000    598.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9414.000
 0.000000000D+00 0.000000000D+00 8.730809152D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.445777846D+04-4.227609187D+01
FeS(c)              Gamma. Pankratz,1987. Chase,1998 pp1241-3 9/77.
 1 g11/00 FE  1.00S   1.00    0.00    0.00    0.00 3   87.9100000     -99621.040
    598.000   1465.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9414.000
-4.651400530D+05 2.845200913D+03 3.227601660D+00 1.639542844D-03-2.119596921D-06
 2.366217205D-09-3.529138060D-13                -3.030024550D+04-3.662233560D+00
FeS(L)              Liquid. Pankratz,1987. Chase,1998 pp1241-3 9/77.
 1 g11/00 FE  1.00S   1.00    0.00    0.00    0.00 4   87.9100000     -99621.040
   1465.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9414.000
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.925935040D+03-3.215631501D+01
FeSO4(cr)           Chase,1998 p1240.
 2 j 6/66 FE  1.00S   1.00O   4.00    0.00    0.00 1  151.9076000    -928848.000
    200.000    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16769.472
-6.203392950D+05 8.502519150D+03-4.378024090D+01 1.731987422D-01-2.431424518D-04
 1.792173046D-07-5.528922570D-11                -1.550636343D+05 2.467116078D+02
    700.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16769.472
-7.679585180D+06 3.308117000D+04-4.678167570D+01 6.781223220D-02-3.741392130D-05
 1.099952323D-08-1.320141816D-12                -3.134827612D+05 3.336437670D+02
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Appendix D (*continued*)

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FeS2(cr)          Pyrite. Chase,1998 p1246.
 2 j 9/77 FE  1.00S   2.00     0.00     0.00     0.00 1  119.9750000    -171544.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9641.000
-2.506864207D+05 3.294827830D+03-1.713873471D+01 8.733851000D-02-1.306227449D-04
 7.362001640D-08 0.000000000D+00                -3.800873290D+04 9.277002410D+01
    600.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9641.000
 9.114353860D+05-5.471736420D+03 2.097363178D+01-1.514620285D-02 1.275975810D-05
-4.881556790D-09 7.710203910D-13                 7.794979850D+03-1.227198763D+02
Fe2O3(cr)         Hematite below Curie pt. Pankratz,1983 p158.
 2 g 1/01 FE  2.00O   3.00     0.00     0.00     0.00 1  159.6882000    -824248.000
    298.150    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-2.713211885D+06 2.323047773D+04-6.765701770D+01 1.306052231D-01-6.970688120D-05
 0.000000000D+00 0.000000000D+00                -2.256089397D+05 4.228072580D+02
    600.000    960.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 3.333492510D+08-1.859961832D+06 3.885138190D+03-3.562599480D+00 1.231055904D-03
 0.000000000D+00 0.000000000D+00                 1.058058870D+07-2.555306055D+04
Fe2O3(cr)         Hematite above Curie pt. Pankratz,1983 p158.
 2 g 1/01 FE  2.00O   3.00     0.00     0.00     0.00 2  159.6882000    -824248.000
    960.000   1800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-2.844009066D+07 1.253786450D+05-2.119080355D+02 2.221481558D-01-1.206765164D-04
 3.480738050D-08-4.165297860D-12                -8.483926520D+05 1.433002161D+03
   1800.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 1.711439880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.041599645D+05-8.780613745D+01
Fe2(SO4)3(cr)     Chase,1998 p1249.
 2 j 6/66 FE  2.00S   3.00O  12.00     0.00     0.00 1  399.8778000   -2582992.400
    298.150    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-3.987499800D+06 4.471584410D+04-1.871627045D+02 5.203843270D-01-5.255167310D-04
 2.053709591D-07 0.000000000D+00                -5.418976280D+05 1.097303717D+03
    700.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-1.749475174D+07 7.308320780D+04-9.392951360D+01 1.468051405D-01-7.963099160D-05
 2.311696556D-08-2.739014918D-12                -7.607146510D+05 6.865330290D+02
Fe3O4(cr)         Magnetite. Pankratz,1983 p160. Westrum,1969.
 3 g 1/01 FE  3.00O   4.00     0.00     0.00     0.00 1  231.5326000    -1118383.200
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           24762.073
-5.182671230D+07 1.293463453D+06-1.341121962D+04 7.401842440D+01-2.285725885D-01
 3.752884300D-04-2.559338368D-07                -5.570751240D+06 6.575689710D+04
    298.150    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           24762.073
-4.407671380D+06 5.351760270D+04-2.613667759D+02 7.431931490D-01-9.767843990D-04
 5.858865440D-07-8.780843180D-11                -4.018075450D+05 1.478276107D+03
    800.000    850.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           24762.073
 0.000000000D+00 0.000000000D+00-1.070116148D+02 1.738436706D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.231022600D+04 6.169265720D+02
Fe3O4(cr)         Magnetite above Curie Pt. Pankratz,1983 p160.
 1 g 1/01 FE  3.00O   4.00     0.00     0.00     0.00 2  231.5326000    -1118383.200
    850.000   1870.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           24762.073
 5.731691980D+07-1.816105186D+05 2.777813396D+02-1.849830315D-01 6.145641150D-05
-3.660350860D-09-1.383713617D-12                 9.906992850D+05-1.868855147D+03
Fe3O4(L)          Liquid. Chase,1998 p1250 6/65.
 1 g 1/01 FE  3.00O   4.00     0.00     0.00     0.00 3  231.5326000    -1118383.200
   1870.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           24762.073
 0.000000000D+00 0.000000000D+00 2.415439996D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.242541349D+05-1.109781572D+02
Ga(cr)            Rhombic. Ref-Elm. Gurvich,1996a pt1 p209 pt2 p169.
 1 tpis96 GA  1.00    0.00     0.00     0.00     0.00 1   69.7230000           0.000
    100.000    302.9207 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5640.000
 1.665524651D+03-1.667535996D+02 3.860876380D+00-1.325442179D-03 2.405494396D-06
 0.000000000D+00 0.000000000D+00                -1.577791876D+02-1.730178030D+01
Ga(L)             Liquid. Ref-Elm. Gurvich,1996a pt1 p209 pt2 p169.
 1 tpis96 GA  1.00    0.00     0.00     0.00     0.00 2   69.7230000           0.000
    302.920   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5640.000
 2.846830421D+04 0.000000000D+00 3.135362156D+00-3.620177256D-05 2.898547239D-08
 0.000000000D+00 0.000000000D+00                -1.716496723D+02-1.053717280D+01
GaBr3(cr)         Gurvich,1996a pt1 p242 pt2 p195.
 1 tpis96 GA  1.00BR  3.00     0.00     0.00     0.00 1  309.4350000     -387000.000
    298.150    397.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           25000.000
 0.000000000D+00 0.000000000D+00 3.563409028D+00 2.798433101D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.885137800D+04-6.997495329D+00
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GaBr3(L)            Liquid. Gurvich,1996a pt1 p242 pt2 p195.
 1 tpis96 GA  1.00BR  3.00    0.00    0.00    0.00 2  309.4350000    -387000.000
    397.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25000.000
 0.000000000D+00 0.000000000D+00 1.544288238D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.990695050D+04-6.330801668D+01
GaCL3(cr)           Triclinic. Gurvich,1996a pt1 p234 pt2 p188.
 1 tpis96 GA  1.00CL  3.00    0.00    0.00    0.00 1  176.0820000    -527000.000
    298.150    351.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20000.000
 0.000000000D+00 0.000000000D+00 2.725476306D+00 2.958442530D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.551070110D+04-8.232857519D+00
GaCL3(L)            Liquid. Gurvich,1996a pt1 p234 pt2 p188.
 1 tpis96 GA  1.00CL  3.00    0.00    0.00    0.00 2  176.0820000    -527000.000
    351.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20000.000
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.599449360D+04-5.489418092D+01
GaF3(cr)            Hexagonal. Gurvich,1996a pt1 p226 pt2 p181.
 1 tpis96 GA  1.00F   3.00    0.00    0.00    0.00 1  126.7182096   -1175000.000
    298.150   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16700.000
 0.000000000D+00 0.000000000D+00 9.361585950D+00 4.503211855D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.443105216D+05-4.313509369D+01
GaI3(cr)            Rhombic. Gurvich,1996a pt1 p249 pt2 p202.
 1 tpis96 GA  1.00I   3.00    0.00    0.00    0.00 1  450.4364100    -218000.000
    298.150    485.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29000.000
 0.000000000D+00 0.000000000D+00 6.461715723D+00 1.866676449D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.897546082D+04-1.772605384D+01
GaI3(L)             Liquid. Gurvich,1996a pt1 p249 pt2 p202.
 1 tpis96 GA  1.00I   3.00    0.00    0.00    0.00 2  450.4364100    -218000.000
    485.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29000.000
 0.000000000D+00 0.000000000D+00 1.656140891D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.012686264D+04-6.793170105D+01
Ga2O3(cr)           Monoclinic. Gurvich,1996a pt1 p219 pt2 p176.
 2 tpis96 GA  2.00O   3.00    0.00    0.00    0.00 1  187.4442000   -1091000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14550.000
-1.515635939D+07 2.787922412D+05-2.090093764D+03 8.236854680D+00-1.771414598D-02
 1.991804320D-05-9.167934200D-09                -1.391968792D+06 1.094221304D+04
    500.000   2080.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14550.000
-2.857534599D+05 0.000000000D+00 1.375883846D+01 1.799504721D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.363570445D+05-7.032081677D+01
Ga2O3(L)            Liquid. Gurvich,1996a pt1 p219 pt2 p176.
 1 tpis96 GA  2.00O   3.00    0.00    0.00    0.00 3  187.4442000   -1091000.000
   2080.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14550.000
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.317078351D+05-1.026657694D+02
Ge(cr)              Cubic. Ref-Elm. Gurvich,1991 pt1 p308 pt2 p268.
 2 tpis91 GE  1.00    0.00    0.00    0.00    0.00 1   72.6400000          0.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4636.360
-2.396506145D+05 3.150572150D+03-1.333941357D+01 3.647997810D-02-2.942104614D-05
 0.000000000D+00 0.000000000D+00                -1.613882957D+04 7.939211600D+01
    400.000   1211.4007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4636.360
-1.888241797D+04 0.000000000D+00 2.898173070D+00 3.591659130D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.433864080D+02-1.298669726D+01
Ge(L)               Liquid. Ref-Elm. Gurvich,1991 pt1 p308 pt2 p268.
 1 tpis91 GE  1.00    0.00    0.00    0.00    0.00 2   72.6400000          0.000
   1211.400   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4636.360
 0.000000000D+00 0.000000000D+00 3.319498082D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 3.278996640D+03-1.185992953D+01
GeO2(II)            Tetragonal Rutile, Gurvich,1991 pt1 p319 pt2 p275.
 2 tpis91 GE  1.00O   2.00    0.00    0.00    0.00 1  104.6388000    -580200.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7230.400
-1.362061010D+04 0.000000000D+00 1.390091028D+00 1.608814892D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.095682740D+04-8.017483700D+00
    298.150   1308.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7230.400
-2.763121338D+05 0.000000000D+00 9.404643208D+00-1.212218158D-03 1.110107511D-06
 0.000000000D+00 0.000000000D+00                -7.346830070D+04-5.004997052D+01
GeO2(I)             Hexagonal alpha-quartz,Gurvich,1991 pt1 p319 pt2 p275.
 1 tpis91 GE  1.00O   2.00    0.00    0.00    0.00 3  104.6388000    -580200.000
   1308.000   1388.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7230.400
-1.535267863D+05 0.000000000D+00 7.481860025D+00 1.711465859D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.994652970D+04-3.711331960D+01
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GeO2(L)             Tetragonal liquid,Gurvich,1991 pt1 p319 pt2 p275.
 1 tpis91 GE  1.00O   2.00     0.00     0.00     0.00 4  104.6388000     -580200.000
   1388.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7230.400
 0.000000000D+00 0.000000000D+00 9.441326067D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.883837870D+04-4.738551165D+01
GeS(cr)             Crystal(II). Gurvich,1991 pt1 p342 pt2 p296.
 2 tpis91 GE  1.00S   1.00     0.00     0.00     0.00 1  104.7050000      -75348.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9657.400
-1.753890915D+04 0.000000000D+00 4.967049230D+00 3.277123440D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.074763864D+04-2.138030847D+01
    298.150    931.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9657.400
 0.000000000D+00 0.000000000D+00 5.015328624D+00 2.453542061D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.066660187D+04-2.131118286D+01
GeS(L)              Liquid. Gurvich,1991 pt1 p342 pt2 p296.
 1 tpis91 GE  1.00S   1.00     0.00     0.00     0.00 3  104.7050000      -75348.000
    931.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9657.400
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.874413010D+03-3.707715519D+01
GeS2(II)            Crystal II. Gurvich,1991 pt1 p345 pt2 p298.
 2 tpis91 GE  1.00S   2.00     0.00     0.00     0.00 1  136.7700000     -121500.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12750.300
-2.239538329D+04 0.000000000D+00 5.754200020D+00 8.048243800D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.676145505D+04-2.405323435D+01
    298.150   1113.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12750.300
-3.367606750D+04 0.000000000D+00 7.889821529D+00 1.310961199D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.713657615D+04-3.427587425D+01
GeS2(L)             Liquid. Gurvich,1991 pt1 p345 pt2 p298.
 1 tpis91 GE  1.00S   2.00     0.00     0.00     0.00 2  136.7700000     -121500.000
   1113.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12750.300
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.893876733D+04-6.006450099D+01
HBO2(cr)            Crystal,metaboric acid. Gurvich,1996a pt1 p41 pt2 p25.
 1 tpis96 H   1.00B   1.00O    2.00     0.00     0.00 1   43.8177400     -804600.000
    298.150    509.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8460.200
 0.000000000D+00 0.000000000D+00 4.478916978D+00 7.045514408D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.841912440D+04-2.172637097D+01
HBO2(L)             Liquid, metaboric acid. Gurvich,1996a pt1 p41 pt2 p25.
 1 tpis96 H   1.00B   1.00O    2.00     0.00     0.00 2   43.8177400     -804600.000
    509.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8460.200
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.993471070D+04-6.555326576D+01
H2O(cr)             Ice. Gordon,1982.
 1 g11/99 H   2.00O   1.00     0.00     0.00     0.00 1   18.0152800     -299108.000
    200.000    273.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
-4.026777480D+05 2.747887946D+03 5.738336630D+01-8.267915240D-01 4.413087980D-03
-1.054251164D-05 9.694495970D-09                 -5.530314990D+04-1.902572063D+02
H2O(L)              Liquid. Cox,1989. Haar,1984. Keenan,1984. Stimson,1969.
 2 g 8/01 H   2.00O   1.00     0.00     0.00     0.00 2   18.0152800     -285830.000
    273.150    373.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13278.000
 1.326371304D+09-2.448295388D+07 1.879428776D+05-7.678995050D+02 1.761556813D+00
-2.151167128D-03 1.092570813D-06                 1.101760476D+08-9.779700970D+05
    373.150    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13278.000
 1.263631001D+09-1.680380249D+07 9.278234790D+04-2.722373950D+02 4.479243760D-01
-3.919397430D-04 1.425743266D-07                 8.113176880D+07-5.134418080D+05
H2SO4(L)            Chase,1998 p1335.
 1 j 9/77 H   2.00S   1.00O    4.00     0.00     0.00 1   98.0784800     -813988.832
    283.456   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          28226.000
-7.749933850D+04 1.040538662D+03 4.433804910D+00 3.648845480D-02-1.743440132D-05
 1.175631937D-08-3.170091690D-12                 -1.068997367D+05-1.353966639D+01
H3BO3(cr)           Triclinic,orthoboric acid. Gurvich,1996a pt1 p48 pt2 p31.
 1 tpis96 H   3.00B   1.00O    3.00     0.00     0.00 1   61.8330200    -1094800.000
    200.000    444.1007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13520.430
 2.370260101D+06-3.116426553D+04 1.488140666D+02-2.710868145D-01 2.274904549D-04
 0.000000000D+00 0.000000000D+00                 1.950811769D+04-8.575441950D+02
H3BO3(L)            Liquid,orthoboric acid. Gurvich,1996a pt1 p48 pt2 p31.
 1 tpis96 H   3.00B   1.00O    3.00     0.00     0.00 2   61.8330200    -1094800.000
    444.100    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13520.430
 0.000000000D+00 0.000000000D+00 2.164890054D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.367426553D+05-1.100910256D+02
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H3PO4(cr)          Crystal,Phosphoric acid. Chase,1998 p1345-7.
 1 j12/71 H   3.00P   1.00O   4.00    0.00    0.00 1   97.9951810   -1284488.000
    200.000    315.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16980.000
 2.733365471D+03 0.000000000D+00 1.109347863D+00 4.129024570D-02-7.810353320D-06
 0.000000000D+00 0.000000000D+00                -1.565753156D+05-4.973473130D+00
H3PO4(L)           Liquid,Phosphoric acid. Chase,1998 pp1345-7.
 1 j12/71 H   3.00P   1.00O   4.00    0.00    0.00 2   97.9951810   -1284488.000
    315.500   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16980.000
 4.109081110D+04-4.410343500D+02 8.547791650D+00 3.198261330D-02 5.167529530D-06
-3.256216600D-09 8.323148740D-13                -1.543175380D+05-4.155398650D+01
Hg(cr)             Tetragonal. Ref-Elm. Chase,1998 pp1373-4.
 1 j12/61 HG  1.00    0.00    0.00    0.00    0.00 1  200.5900000          0.000
    100.000    234.2907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9343.000
-3.184586610D+03 0.000000000D+00 3.464424870D+00-4.054864610D-03 1.766281131D-05
 0.000000000D+00 0.000000000D+00                -1.282454336D+03-1.132010161D+01
Hg(L)              Liquid. Ref-Elm. Chase,1998 pp1373-4.
 2 j12/61 HG  1.00    0.00    0.00    0.00    0.00 2  200.5900000          0.000
    234.290    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9343.000
 1.058325418D+05-1.993826150D+03 1.880577074D+01-5.994680920D-02 1.228327030D-04
-1.293155349D-07 5.530734430D-11                7.916778390D+03-9.064871100D+01
    600.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9343.000
 7.913840080D+05-3.956327060D+03 1.106465862D+01-8.153982650D-03 4.970504160D-06
-1.510428227D-09 1.872051162D-13                2.213772421D+04-6.072461670D+01
HgBr2(cr)          Chase,1998 p482 3/62. Pankratz,1984 p302.
 1 g12/00 HG  1.00BR  2.00    0.00    0.00    0.00 1  360.3980000    -175309.600
    298.150    514.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-1.853158540D+06 2.003808568D+04-7.235875200D+01 1.451267662D-01-9.240269430D-05
 0.000000000D+00 0.000000000D+00                -1.255295454D+05 4.503769710D+02
HgBr2(L)           Chase,1998 pp482-4 3/62.
 1 g12/00 HG  1.00BR  2.00    0.00    0.00    0.00 2  360.3980000    -175309.600
    514.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 1.227853475D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.320342036D+04-4.684603799D+01
HgO(cr)            Chase,1998 p1382.
 2 j 6/62 HG  1.00O   1.00    0.00    0.00    0.00 1  216.5894000     -90789.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9104.000
-1.062935837D+04 0.000000000D+00 3.345782860D+00 8.775373380D-03-6.110417750D-06
 0.000000000D+00 0.000000000D+00                -1.228859467D+04-1.301600791D+01
    400.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9104.000
 1.582008299D+06-1.511620794D+04 6.157172990D+01-1.075963114D-01 1.203602940D-04
-7.037671400D-08 1.672097585D-11                6.599870400D+04-3.568628600D+02
I2(cr)             Rhombic. Ref-Elm. Gurvich,1989 pt1 p219 pt2 p315.
 1 tpis89 I   2.00    0.00    0.00    0.00    0.00 1  253.8089400          0.000
    200.000    386.7507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13196.000
-3.901269140D+06 9.143202330D+04-8.900457500D+02 4.671270160D+00-1.357161837D-02
 2.073947355D-05-1.292905191D-08                -3.912632630D+05 4.422603650D+03
I2(L)              Liquid. Ref-Elm. Gurvich,1989 pt1 p219 pt2 p315.
 1 tpis89 I   2.00    0.00    0.00    0.00    0.00 2  253.8089400          0.000
    386.750   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13196.000
 0.000000000D+00 0.000000000D+00 9.568212679D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.204453805D+03-3.637326088D+01
In(cr)             Tetragonal. Ref-Elm. Gurvich,1996a pt1 255 pt2 p207.
 1 tpis96 IN  1.00    0.00    0.00    0.00    0.00 1  114.8180000          0.000
    100.000    429.7847 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6610.080
 8.511616870D+03-3.450470040D+02 6.838785170D+00-1.818530679D-02 4.122421420D-05
-2.960008730D-08 0.000000000D+00                4.580589980D+02-2.928914154D+01
In(L)              Liquid. Ref-Elm. Gurvich,1996a pt1 255 pt2 p207.
 1 tpis96 IN  1.00    0.00    0.00    0.00    0.00 2  114.8180000          0.000
    429.784   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6610.080
 5.092302493D+04 0.000000000D+00 3.302178962D+00-1.313366633D-04 6.037637816D-08
 0.000000000D+00 0.000000000D+00                -4.511517590D+02-1.075015830D+01
InBr(cr)           Rhombic Gurvich,1996a pt1 p289 pt2 p232.
 1 tpis96 IN  1.00BR  1.00    0.00    0.00    0.00 1  194.7220000    -175000.000
    298.150    558.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12200.000
 0.000000000D+00 0.000000000D+00 4.633586345D+00 4.628534935D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.263476911D+04-1.455042037D+01
InBr(L)            Liquid Gurvich,1996a pt1 p289 pt2 p232
 1 tpis96 IN  1.00BR  1.00    0.00    0.00    0.00 2  194.7220000    -175000.000
    558.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12200.000
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.222238473D+04-3.267500998D+01
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InBr3(cr)          Gurvich,1996a pt1 p292 pt2 p235.
 1 tpis96 IN  1.00BR  3.00     0.00     0.00     0.00 1  354.5300000     -399000.000
    298.150    693.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24500.000
 0.000000000D+00 0.000000000D+00 1.154114915D+01 2.436824299D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.153769860D+04-4.543581045D+01
InBr3(L)           Liquid Gurvich,1996a pt1 p292 pt2 p235.
 1 tpis96 IN  1.00BR  3.00     0.00     0.00     0.00 2  354.5300000     -399000.000
    693.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24500.000
 0.000000000D+00 0.000000000D+00 1.623667540D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.107949370D+04-6.994831229D+01
InCL(crII)         Cubic Gurvich,1996a pt1 p280 pt2 p224.
 1 tpis96 IN  1.00CL  1.00     0.00     0.00     0.00 1  150.2710000     -186500.000
    298.150    387.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12400.000
 0.000000000D+00 0.000000000D+00 5.163984408D+00 3.438567035D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.412314134D+04-1.842034240D+01
InCL(crI)          Rhombic Gurvich,1996a pt1 p280 pt2 p224.
 1 tpis96 IN  1.00CL  1.00     0.00     0.00     0.00 2  150.2710000     -186500.000
    387.000    484.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12400.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.441117035D+04-2.629006183D+01
InCL(L)            Liquid Gurvich,1996a pt1 p280 pt2 p224
 1 tpis96 IN  1.00CL  1.00     0.00     0.00     0.00 3  150.2710000     -186500.000
    484.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12400.000
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.248971016D+04-2.917594080D+01
InCl3(cr)          Monoclinic Gurvich,1996a pt1 p284 pt2 p227.
 1 tpis96 IN  1.00CL  3.00     0.00     0.00     0.00 1  221.1770000     -530000.000
    298.150    856.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21000.000
 0.000000000D+00 0.000000000D+00 1.093437857D+01 3.665158861D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.716697410D+04-4.631386948D+01
InCl3(L)           Liquid Gurvich,1996a pt1 p284 pt2 p227.
 1 tpis96 IN  1.00CL  3.00     0.00     0.00     0.00 2  221.1770000     -530000.000
    856.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          21000.000
 0.000000000D+00 0.000000000D+00 1.407178535D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.526246230D+04-6.056749656D+01
InF3(cr)           Hexagonal Gurvich,1996a pt1 p274 pt2 p219.
 1 tpis96 IN  1.00F   3.00     0.00     0.00     0.00 1  171.8132096    -1190000.000
    298.150   1445.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19400.000
 0.000000000D+00 0.000000000D+00 9.751747247D+00 4.404348542D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.462265291D+05-4.364479594D+01
InF3(L)            Liquid Gurvich,1996a pt1 p274 pt2 p219.
 1 tpis96 IN  1.00F   3.00     0.00     0.00     0.00 2  171.8132096    -1190000.000
   1445.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19400.000
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.431278760D+05-7.826197980D+01
InI(cr)            Rhombic Gurvich,1996a pt1 p296 pt2 p240
 1 tpis96 IN  1.00I   1.00     0.00     0.00     0.00 1  241.7224700     -102500.000
    200.000    637.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13354.000
-9.253976720D+04 1.215133840D+03-1.038882859D-02 1.368794477D-02-9.117964390D-06
 1.596277777D-09 1.519819589D-12                 -2.009017203D+04 1.436598613D+01
InI(L)             Liquid Gurvich,1996a pt1 p296 pt2 p240
 1 tpis96 IN  1.00I   1.00     0.00     0.00     0.00 2  241.7224700     -102500.000
    637.500   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13354.000
 0.000000000D+00 0.000000000D+00 8.443071209D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.331949891D+04-3.168475714D+01
InI2(crII)         Gurvich,1996a pt1 p299 pt2 p242.
 1 tpis96 IN  1.00I   2.00     0.00     0.00     0.00 1  368.6269400     -176000.000
    200.000    428.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19197.000
 2.657410907D+04 0.000000000D+00 6.946210170D+00 6.889884760D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.345592914D+04-2.056620828D+01
InI2(crI)          Gurvich,1996a pt1 p299 pt2 p242.
 1 tpis96 IN  1.00I   2.00     0.00     0.00     0.00 2  368.6269400     -176000.000
    428.000    497.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19197.000
 0.000000000D+00 0.000000000D+00 1.080520680D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.438345996D+04-4.070950647D+01
InI2(L)            Liquid Gurvich,1996a pt1 p299 pt2 p242.
 1 tpis96 IN  1.00I   2.00     0.00     0.00     0.00 3  368.6269400     -176000.000
    497.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19197.000
 0.000000000D+00 0.000000000D+00 1.379516051D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.444424767D+04-5.640525880D+01
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InI3(cr)          Monoclinic Gurvich,1996a pt1 p301 pt2 p244.
 1 tpis96 IN  1.00I   3.00    0.00    0.00    0.00 1  495.5314100    -224000.000
    296.000    480.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29888.000
-1.888265213D+03 0.000000000D+00 1.096468704D+01 4.804492387D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.042985260D+04-3.708283570D+01
InI3(L)           Liquid Gurvich,1996a pt1 p301 pt2 p244.
 1 tpis96 IN  1.00I   3.00    0.00    0.00    0.00 2  495.5314100    -224000.000
    480.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         29888.000
 0.000000000D+00 0.000000000D+00 1.652532741D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.031892811D+04-6.447232654D+01
In2O3(cr)         Cubic. Gurvich,1996a pt1 p267 pt2 p214.
 2 tpis96 IN  2.000   3.00    0.00    0.00    0.00 1  277.6342000    -923000.000
    200.000     500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16600.000
-9.503707350D+06 1.770907496D+05-1.344503703D+03 5.391303710D+00-1.171772659D-02
 1.329195789D-05-6.163943540D-09                -9.104733670D+05 7.021339210D+03
    500.000    2186.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16600.000
-2.719943809D+05 0.000000000D+00 1.461433085D+01 1.210173540D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.163340719D+05-7.291389772D+01
In2O3(L)          Liquid.  Gurvich,1996a pt1 p267 pt2 p214.
 1 tpis96 IN  2.000   3.00    0.00    0.00    0.00 2  277.6342000    -923000.000
   2186.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16600.000
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.108089477D+05-1.000602622D+02
K(cr)             Cubic. Ref-Elm. Cox,1989 p257.
 1 coda89 K   1.00    0.00    0.00    0.00    0.00 1   39.0983000          0.000
    200.000    336.8607 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7088.000
-1.022031747D+05 0.000000000D+00 1.333752016D+01-5.580990750D-02 9.013009100D-05
 0.000000000D+00 0.000000000D+00                -2.635062430D+03-5.615376520D+01
K(L)              Liquid. Ref-Elm. Cox,1989 p257.
 1 coda89 K   1.00    0.00    0.00    0.00    0.00 2   39.0983000          0.000
    336.860   2200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          7088.000
-3.935722030D+03-4.547278110D+01 4.845244000D+00-3.083546588D-03 2.015548866D-06
-3.706172930D-11 5.032895480D-15                -8.075609680D+02-1.836641748D+01
KALO2(II)         Cubic  Gurvich,1982 pt1 p416 pt2 p440.
 2 tpis82 K   1.00AL  1.00O   2.00    0.00    0.00 1   98.0786380   -1130600.000
    200.000     500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13355.000
-4.112581400D+06 7.776836810D+04-5.971614160D+02 2.439288137D+00-5.340052400D-03
 6.098541950D-06-2.843205389D-09                -4.867714660D+05 3.112191530D+03
    500.000     810.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13355.000
-1.565945988D+05 0.000000000D+00 9.609859180D+00 4.379778490D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.395641536D+05-4.665045360D+01
KALO2(I)          Cubic  Gurvich,1982 pt1 p416 pt2 p440.
 1 tpis82 K   1.00AL  1.00O   2.00    0.00    0.00 2   98.0786380   -1130600.000
    810.000    1986.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13355.000
 8.202527870D+05 0.000000000D+00 7.962706161D+00 3.725414967D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.366535595D+05-3.415265795D+01
KALO2(L)          Liquid. Gurvich,1982 pt1 p416 pt2 p440.
 1 tpis82 K   1.00AL  1.00O   2.00    0.00    0.00 3   98.0786380   -1130600.000
   1986.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13355.000
 0.000000000D+00 0.000000000D+00 1.563531705D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.350952219D+05-8.015693620D+01
KBO2(cr)          Hexagonal. Gurvich,1982 pt1 p414 pt2 p438.
 2 tpis82 K   1.00B   1.00O   2.00    0.00    0.00 1   81.9081000    -983000.000
    200.000     500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12114.000
-1.601790683D+07 2.997219831D+05-2.274223151D+03 9.014942220D+00-1.951702277D-02
 2.207384968D-05-1.021270864D-08                -1.468642542D+06 1.188723021D+04
    500.000    1220.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12114.000
-2.328709444D+05 0.000000000D+00 9.862977090D+00 2.740064145D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.220704116D+05-4.870043770D+01
KBO2(L)           Liquid. Gurvich,1982 pt1 p414 pt2 p438.
 1 tpis82 K   1.00B   1.00O   2.00    0.00    0.00 2   81.9081000    -983000.000
   1220.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12114.000
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.250545034D+05-9.581938648D+01
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KBr(cr)            Cubic. Gurvich,1982 pt1 p394 pt2 p422.
 2 tpis82 K   1.00BR  1.00     0.00     0.00     0.00 1  119.0023000     -393450.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12210.000
 5.931068110D+06-1.101548735D+05 8.346526100D+02-3.241060370D+00 6.976184850D-03
-7.847251340D-06 3.614707700D-09                 4.475606580D+05-4.361638690D+03
    500.000   1007.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12210.000
 3.145485337D+04 0.000000000D+00 5.199966220D+00 2.540382104D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.887872000D+04-1.867132005D+01
KBr(L)             Liquid. Gurvich,1982 pt1 p394 pt2 p422.
 1 tpis82 K   1.00BR  1.00     0.00     0.00     0.00 2  119.0023000     -393450.000
   1007.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12210.000
 0.000000000D+00 0.000000000D+00 8.358881040D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.773361440D+04-3.492371367D+01
KCN(II)            Chase,1998 pp617-9.
 2 j 3/66 K   1.00C   1.00N   1.00     0.00     0.00 1   65.1157000     -113470.000
    168.300    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17343.000
 4.789226660D+04-6.869399420D+02 1.189656301D+01-9.957932230D-03 9.253758250D-06
 0.000000000D+00 0.000000000D+00                -1.275880363D+04-5.189047360D+01
    400.000    895.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17343.000
-8.550726080D+04 7.115109180D+02 5.642442360D+00 3.733592200D-03-2.880609857D-06
 8.848387980D-10 0.000000000D+00                -1.981154134D+04-1.586461470D+01
KCN(L)             Chase,1998 pp617-9.
 1 j 3/66 K   1.00C   1.00N   1.00     0.00     0.00 2   65.1157000     -113470.000
    895.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17343.000
 0.000000000D+00 0.000000000D+00 9.057899984D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.522666331D+04-3.545330543D+01
KCL(cr)            Cubic. Gurvich,1982 pt1 p390 pt2 p419.
 2 tpis82 K   1.00CL  1.00     0.00     0.00     0.00 1   74.5513000     -436490.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11370.000
 1.179895024D+06-2.217824961D+04 1.730930630D+02-6.545434150D-01 1.415897824D-03
-1.598259237D-06 7.387534150D-10                 4.560782730D+04-8.991527150D+02
    500.000   1044.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11370.000
 2.888789664D+02 0.000000000D+00 5.287088550D+00 4.004092160D-03-4.343449010D-06
 2.753186288D-09 0.000000000D+00                -5.421785640D+04-2.121648362D+01
KCL(L)             Liquid. Gurvich,1982 pt1 p390 pt2 p419.
 1 tpis82 K   1.00CL  1.00     0.00     0.00     0.00 2   74.5513000     -436490.000
   1044.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11370.000
 0.000000000D+00 0.000000000D+00 8.659560215D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.322113230D+04-3.876839685D+01
KF(cr)             Cubic. Gurvich,1982 pt1 p387 pt2 p416.
 2 tpis82 K   1.00F   1.00     0.00     0.00     0.00 1   58.0967032     -569900.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10000.000
-2.920039956D+06 5.319604560D+04-3.910182930D+02 1.542524798D+00-3.296460120D-03
 3.692487030D-06-1.695192481D-09                 -3.107774664D+05 2.055199175D+03
    500.000   1131.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10000.000
-3.379466710D+04 0.000000000D+00 5.806099490D+00 1.562870483D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.045670350D+04-2.573881635D+01
KF(L)              Liquid. Gurvich,1982 pt1 p387 pt2 p416.
 1 tpis82 K   1.00F   1.00     0.00     0.00     0.00 2   58.0967032     -569900.000
   1131.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10000.000
 0.000000000D+00 0.000000000D+00 8.455098376D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.905565270D+04-3.960518579D+01
KH(cr)             Cubic. Gurvich,1982 pt1 p381 pt2 p411.
 1 tpis82 K   1.00H   1.00     0.00     0.00     0.00 1   40.1062400      -57820.000
    298.150    892.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7800.000
-6.457385920D+04 0.000000000D+00 4.092965190D+00 3.996988400D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.568660280D+03-1.870503989D+01
KH(L)              Liquid. Gurvich,1982 pt1 p381 pt2 p411.
 1 tpis82 K   1.00H   1.00     0.00     0.00     0.00 2   40.1062400      -57820.000
    892.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7800.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.737318610D+03-3.021766413D+01
K(HF2)(a)          Alpha.  Chase,1998 pp1104-6.
 1 j 6/71 K   1.00H   1.00F   2.00     0.00     0.00 1   78.1030464     -931232.880
    200.000    469.8507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15294.000
 2.015718998D+03-3.533789190D+02 8.928247670D+00 2.814397451D-03 7.299809050D-06
 0.000000000D+00 0.000000000D+00                -1.128323001D+05-4.066701520D+01
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K(HF2)(b)          Beta.    Chase,1998 pp1104-6.
 1 j 6/71 K   1.00H   1.00F   2.00    0.00    0.00 2   78.1030464    -931232.880
    469.850    511.9507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15294.000
 0.000000000D+00 0.000000000D+00 1.205711461D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.145682138D+05-5.416912090D+01
K(HF2)(L)          Liquid. Chase,1998 pp1104-6.
 1 j 6/71 K   1.00H   1.00F   2.00    0.00    0.00 3   78.1030464    -931232.880
    511.950   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15294.000
 0.000000000D+00 0.000000000D+00 1.258041665D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.140400401D+05-5.587860571D+01
KI(cr)             Cubic. Gurvich,1982 pt1 p398 pt2 p425.
 2 tpis82 K   1.00I   1.00    0.00    0.00    0.00 1  166.0027700    -329300.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12700.000
 3.849118670D+06-7.198411950D+04 5.507582640D+02-2.141022674D+00 4.628312070D-03
-5.222322770D-06 2.411694600D-09                 2.826852967D+05-2.871024327D+03
    500.000    954.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12700.000
 2.770577458D+04 0.000000000D+00 5.235901210D+00 2.694044229D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.119339520D+04-1.772462446D+01
KI(L)              Liquid. Gurvich,1982 pt1 p398 pt2 p425.
 1 tpis82 K   1.00I   1.00    0.00    0.00    0.00 2  166.0027700    -329300.000
    954.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12700.000
 0.000000000D+00 0.000000000D+00 8.455098376D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.017867910D+04-3.422733253D+01
KNO2(II)           Hexagonal. Gurvich,1982 pt1 p404 pt2 p430.
 1 tpis82 K   1.00N   1.00O   2.00    0.00    0.00 1   85.1038000    -365900.000
    200.000    314.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22940.000
-1.228297484D+07 0.000000000D+00 1.182559906D+03-6.076842320D+00 8.778424840D-03
 0.000000000D+00 0.000000000D+00                -2.452424942D+05-5.366905900D+03
KNO2(I)            Cubic. Gurvich,1982 pt1 p404 pt2 p430.
 1 tpis82 K   1.00N   1.00O   2.00    0.00    0.00 2   85.1038000    -365900.000
    314.700    711.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22940.000
 0.000000000D+00 0.000000000D+00 9.827879214D+00 2.012866663D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.687774970D+04-3.782318671D+01
KNO2(L)            Liquid. Gurvich,1982 pt1 p404 pt2 p430.
 1 tpis82 K   1.00N   1.00O   2.00    0.00    0.00 3   85.1038000    -365900.000
    711.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22940.000
 0.000000000D+00 0.000000000D+00 1.226771030D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.609515960D+04-4.958866367D+01
KNO3(a)            Rhombic. Gurvich,1982 pt1 p407 pt2 p432.
 1 tpis82 K   1.00N   1.00O   3.00    0.00    0.00 1  101.1032000    -494000.000
    200.000    402.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18750.000
 3.565624070D+06-6.291319380D+04 4.392599940D+02-1.436497824D+00 2.380417773D-03
-1.518208824D-06 0.000000000D+00                 2.258505778D+05-2.341795728D+03
KNO3(b)            Hexagonal. Gurvich,1982 pt1 p407 pt2 p432.
 1 tpis82 K   1.00N   1.00O   3.00    0.00    0.00 2  101.1032000    -494000.000
    402.000    607.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18750.000
 3.211975210D+06 0.000000000D+00-5.032659772D+01 1.462070525D-01-8.159374395D-05
 0.000000000D+00 0.000000000D+00                -3.934846620D+04 2.807123740D+02
KNO3(L)            Liquid. Gurvich,1982 pt1 p407 pt2 p432.
 1 tpis82 K   1.00N   1.00O   3.00    0.00    0.00 3  101.1032000    -494000.000
    607.700   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18750.000
 0.000000000D+00 0.000000000D+00 1.695830542D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.345106350D+04-7.918784042D+01
KOH(a)             Alpha,beta. Gurvich,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00    0.00    0.00 1   56.1056400    -423400.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12600.000
-4.380064620D+05 1.125472885D+04-1.023623342D+02 4.375630440D-01-5.920346390D-04
 0.000000000D+00 0.000000000D+00                -1.002155756D+05 5.241308280D+02
KOH(b)             Beta.       Gurvich,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00    0.00    0.00 2   56.1056400    -423400.000
    298.150    517.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12600.000
-2.814357070D+03 0.000000000D+00 6.478313214D+00 6.183767895D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.313882160D+04-2.899826328D+01
KOH(c)             Gamma.      Gurvich,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00    0.00    0.00 3   56.1056400    -423400.000
    517.000    679.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12600.000
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.325857830D+04-4.413346659D+01
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Appendix D (*continued*)

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KOH(L)              Liquid.     Gurvich,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00     0.00     0.00 4    56.1056400     -423400.000
    679.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12600.000
 0.000000000D+00 0.000000000D+00 1.046363526D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.288008340D+04-4.822385687D+01
KO2(b)              Tetragonal. Gurvich,1982 pt1 p375 pt2 p405.
 1 tpis82 K   1.00O   2.00     0.00     0.00     0.00 1    71.0971000     -283600.000
    200.000    422.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16820.000
 5.149174260D+06-7.614604350D+04 4.537181540D+02-1.295601160D+00 1.892822220D-03
-1.090404806D-06 0.000000000D+00                 3.247518810D+05-2.484666478D+03
KO2(a)              Cubic. Gurvich,1982 pt1 p375 pt2 p405.
 1 tpis82 K   1.00O   2.00     0.00     0.00     0.00 2    71.0971000     -283600.000
    422.000    808.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16820.000
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.734259730D+04-4.545206851D+01
KO2(L)              Liquid. Gurvich,1982 pt1 p375 pt2 p405.
 1 tpis82 K   1.00O   2.00     0.00     0.00     0.00 3    71.0971000     -283600.000
    808.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16820.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.603115500D+04-5.204773022D+01
K2CO3(a)            Monoclinic. Gurvich,1982 pt1 p410 pt2 p434.
 1 tpis82 K   2.00C   1.00O   3.00     0.00     0.00 1   138.2055000    -1151500.000
    200.000    693.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22665.000
-3.632826430D+05 5.957567840D+03-3.080710797D+01 1.494558714D-01-2.377158989D-04
 2.231711601D-07-8.466662880D-11                -1.694136603D+05 1.763682121D+02
K2CO3(b)            Hexagonal. Gurvich,1982 pt1 p410 pt2 p434.
 1 tpis82 K   2.00C   1.00O   3.00     0.00     0.00 2   138.2055000    -1151500.000
    693.000   1173.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22665.000
 0.000000000D+00 0.000000000D+00 1.310023080D+01 8.280944999D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.424065852D+05-5.805609552D+01
K2CO3(L)            Liquid. Gurvich,1982 pt1 p410 pt2 p434.
 1 tpis82 K   2.00C   1.00O   3.00     0.00     0.00 3   138.2055000    -1151500.000
   1173.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22665.000
 0.000000000D+00 0.000000000D+00 2.471582811D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.466663988D+05-1.273064200D+02
K2O(c)              III Cubic. Gurvich,1982 pt1 p377 pt2 p406.
 1 tpis82 K   2.00O   1.00     0.00     0.00     0.00 1    94.1960000     -361700.000
    298.150    590.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13700.000
 0.000000000D+00 0.000000000D+00 6.140710637D+00 8.448122619D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.570860710D+04-2.596002023D+01
K2O(b)              II Cubic. Gurvich,1982 pt1 p377 pt2 p406.
 1 tpis82 K   2.00O   1.00     0.00     0.00     0.00 2    94.1960000     -361700.000
    590.000    645.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13700.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.762703040D+04-5.838924536D+01
K2O(a)              I Tetragonal. Gurvich,1982 pt1 p377 pt2 p406.
 1 tpis82 K   2.00O   1.00     0.00     0.00     0.00 3    94.1960000     -361700.000
    645.000   1013.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13700.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.714594370D+04-5.764337454D+01
K2O(L)              Liquid. Gurvich,1982 pt1 p377 pt2 p406.
 1 tpis82 K   2.00O   1.00     0.00     0.00     0.00 4    94.1960000     -361700.000
   1013.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13700.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.389860860D+04-5.443771306D+01
K2O2(cr)            Rhombic. Gurvich,1982 pt1 p379 pt2 p409.
 1 tpis82 K   2.00O   2.00     0.00     0.00     0.00 1   110.1954000     -443000.000
    298.150    818.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17000.000
 0.000000000D+00 0.000000000D+00 9.151230800D+00 6.015267286D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.627614800D+04-3.986168914D+01
K2O2(L)             Liquid. Gurvich,1982 pt1 p379 pt2 p409.
 1 tpis82 K   2.00O   2.00     0.00     0.00     0.00 2   110.1954000     -443000.000
    818.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17000.000
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.749561030D+04-7.864151320D+01
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K2S(cr)           Below lambda. Chase,1998 pp1486-8.
 2 j 3/78 K   2.00S   1.00     0.00     0.00     0.00 1  110.2616000    -376560.000
    298.150    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 4.724669150D+04-4.465995260D+02 9.600035840D+00 7.836273870D-04 1.295338974D-06
 0.000000000D+00 0.000000000D+00                -4.549501380D+04-4.238203950D+01
    600.000   1050.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 1.237549376D+09-7.863379810D+06 1.968151557D+04-2.415909047D+01 1.451020806D-02
-3.388041040D-06 0.000000000D+00                4.392639800D+07-1.251401185D+05
K2S(cr)           Above lambda. Chase,1998 pp1486-8.
 2 j 3/78 K   2.00S   1.00     0.00     0.00     0.00 2  110.2616000    -376560.000
   1050.000   1100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 1.564212060D+02-1.266383838D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.311392922D+05-9.279088390D+02
   1100.000   1221.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 1.711898382D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.452307000D+04-9.166848070D+01
K2S(L)            Chase,1998 pp1486-8.
 1 j 3/78 K   2.00S   1.00     0.00     0.00     0.00 3  110.2616000    -376560.000
   1221.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 1.214261815D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.650451120D+04-5.470849197D+01
K2SO4(II)         Rhombic. Gurvich,1982 pt1 p402 pt2 p428.
 2 tpis82 K   2.00S   1.00O    4.00     0.00     0.00 1  174.2592000   -1437700.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25435.000
 7.718871240D+06-1.416712413D+05 1.060181562D+03-4.031007910D+00 8.614683760D-03
-9.611228510D-06 4.397898620D-09                4.640403120D+05-5.555950140D+03
    500.000    857.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25435.000
-4.858415070D+04 0.000000000D+00 1.165680854D+01 1.576835485D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.772539211D+05-5.027549500D+01
K2SO4(I)          Hexagonal. Gurvich,1982 pt1 p402 pt2 p428.
 1 tpis82 K   2.00S   1.00O    4.00     0.00     0.00 2  174.2592000   -1437700.000
    857.000   1342.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25435.000
 1.683008379D+07 0.000000000D+00-3.453625048D+01 4.086410384D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.262250083D+05 2.527928284D+02
K2SO4(L)          Liquid. Gurvich,1982 pt1 p402 pt2 p428.
 1 tpis82 K   2.00S   1.00O    4.00     0.00     0.00 3  174.2592000   -1437700.000
   1342.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         25435.000
 0.000000000D+00 0.000000000D+00 2.405433393D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.762313671D+05-1.157513010D+02
K2SiO3(cr)        Rhombic. Gurvich,1982 pt1 p412 pt2 p436.
 2 tpis82 K   2.00SI  1.00O    3.00     0.00     0.00 1  154.2803000   -1543000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21860.000
 2.855673428D+06-5.059971270D+04 3.647712840D+02-1.277216470D+00 2.614874944D-03
-2.812883261D-06 1.248415754D-09                4.217450990D+04-1.927446205D+03
    500.000   1249.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21860.000
-1.541934726D+05 0.000000000D+00 1.400996506D+01 6.254878280D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.905514472D+05-6.499565930D+01
K2SiO3(L)         Liquid. Gurvich,1982 pt1 p412 pt2 p436.
 1 tpis82 K   2.00SI  1.00O    3.00     0.00     0.00 2  154.2803000   -1543000.000
   1249.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21860.000
 0.000000000D+00 0.000000000D+00 2.285161723D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.941869756D+05-1.182498589D+02
K2Si2O5(a)        III. Gurvich,1982 pt1 p413 pt2 p437.
 1 tpis82 K   2.00SI  2.00O    5.00     0.00     0.00 1  214.3646000   -2505000.000
    200.000    510.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28820.000
-1.332332468D+07 2.509615155D+05-1.911732601D+03 7.658564980D+00-1.652056677D-02
 1.854450564D-05-8.489711240D-09                -1.432942804D+06 9.985815260D+03
K2Si2O5(b)        II. Gurvich,1982 pt1 p413 pt2 p437.
 1 tpis82 K   2.00SI  2.00O    5.00     0.00     0.00 2  214.3646000   -2505000.000
    510.000    867.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28820.000
-1.201153165D+05 0.000000000D+00 1.900352516D+01 1.092379467D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.078422822D+05-8.941094441D+01
K2Si2O5(c)        I. Gurvich,1982 pt1 p413 pt2 p437.
 1 tpis82 K   2.00SI  2.00O    5.00     0.00     0.00 3  214.3646000   -2505000.000
    867.000   1318.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         28820.000
 0.000000000D+00 0.000000000D+00 2.696791513D+01 5.313602365D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.105104930D+05-1.339782607D+02
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K2Si2O5(L)          Gurvich,1982 pt1 p413 pt2 p437.
 1 tpis82 K   2.00SI  2.00O   5.00     0.00     0.00 4  214.3646000   -2505000.000
   1318.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          28820.000
 0.000000000D+00 0.000000000D+00 3.307470915D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.138641654D+05-1.739362353D+02
K3ALF6(II)          Tetragonal. Gurvich,1982 pt1 p418 pt2 p442.
 1 tpis82 K   3.00AL  1.00F   6.00     0.00     0.00 1  258.2668572   -3347000.000
    298.150    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          42600.000
 0.000000000D+00 0.000000000D+00 1.838593014D+01 2.828982105D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.092884330D+05-7.891279947D+01
K3ALF6(I)           Cubic. Gurvich,1982 pt1 p418 pt2 p442.
 1 tpis82 K   3.00AL  1.00F   6.00     0.00     0.00 2  258.2668572   -3347000.000
    600.000   1273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          42600.000
 0.000000000D+00 0.000000000D+00 2.893014742D+01 6.707551016D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.109483890D+05-1.321111106D+02
K3ALF6(L)           Liquid. Gurvich,1982 pt1 p418 pt2 p442.
 1 tpis82 K   3.00AL  1.00F   6.00     0.00     0.00 3  258.2668572   -3347000.000
   1273.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          42600.000
 0.000000000D+00 0.000000000D+00 4.726676617D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.141107070D+05-2.430801826D+02
Li(cr)              Crystal. Ref-Elm. Gurvich,1982 pt1 p245 pt2 p286.
 2 tpis82 LI  1.00    0.00    0.00     0.00     0.00 1    6.9410000          0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4632.000
-9.860652350D+03 0.000000000D+00 2.304323850D+00 2.671663720D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.388536120D+02-1.047881686D+01
    298.150    453.6907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4632.000
 7.238824960D+04 0.000000000D+00 1.570314469D-01 6.770404110D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.049497436D+02 9.961763140D-01
Li(L)               Liquid. Ref-Elm. Gurvich,1982 pt1 p245 pt2 p286.
 1 tpis82 LI  1.00    0.00    0.00     0.00     0.00 2    6.9410000          0.000
    453.690   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4632.000
 2.465569228D+04 0.000000000D+00 3.755723428D+00-6.332303407D-04 3.160739478D-07
 0.000000000D+00 0.000000000D+00                -7.299116690D+02-1.701274654D+01
LiALO2(cr)          Chase,1998 pp126-8.
 2 j12/79 LI  1.00AL  1.00O   2.00     0.00     0.00 1   65.9213380   -1188674.400
    200.000    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9694.328
-2.403553110D+06 4.191135380D+04-2.947543676D+02 1.096024513D+00-2.070932308D-03
 1.989368601D-06-7.643124070D-10                -3.359272460D+05 1.562056779D+03
    700.000   1973.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9694.328
-1.440922218D+06 5.833386140D+03-1.030268470D+00 1.461691077D-02-7.831786240D-06
 2.428705700D-09-3.067767899D-13                -1.811607791D+05 2.012864902D+01
LiALO2(L)           Chase,1998 pp126-8.
 1 j12/79 LI  1.00AL  1.00O   2.00     0.00     0.00 2   65.9213380   -1188674.400
   1973.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9694.328
 0.000000000D+00 0.000000000D+00 1.509649997D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.416553963D+05-8.099434263D+01
LiBO2(cr)           Monoclinic. Gurvich,1982 pt1 p298 pt2 p331.
 2 tpis82 LI  1.00B   1.00O   2.00     0.00     0.00 1   49.7508000   -1022900.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8880.000
-1.298972763D+02 2.476112547D+03-4.025475640D+01 2.755313951D-01-7.202835830D-04
 9.355885600D-07-4.776147920D-10                -1.326385762D+05 1.863684915D+02
    500.000   1122.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8880.000
-1.501059611D+05 0.000000000D+00 7.094387770D+00 5.990864950D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.259108022D+05-3.688511780D+01
LiBO2(L)            Liquid. Gurvich,1982 pt1 p298 pt2 p331.
 1 tpis82 LI  1.00B   1.00O   2.00     0.00     0.00 2   49.7508000   -1022900.000
   1122.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8880.000
 0.000000000D+00 0.000000000D+00 1.736722910D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.294550343D+05-9.861468152D+01
LiBr(cr)            Cubic. Gurvich,1982 pt1 p284 pt2 p317.
 2 tpis82 LI  1.00BR  1.00    0.00     0.00     0.00 1   86.8450000    -351160.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10476.000
 3.743262690D+06-7.020131930D+04 5.366833500D+02-2.085864954D+00 4.508762520D-03
-5.086004120D-06 2.348146084D-09                2.721051038D+05-2.801510974D+03
    500.000    823.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10476.000
 1.459008908D+04 0.000000000D+00 4.895008630D+00 3.134322823D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.378446420D+04-1.984092688D+01
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LiBr(L)           Liquid. Gurvich,1982 pt1 p284 pt2 p317.
 1 tpis82 LI  1.00BR  1.00    0.00    0.00    0.00 2   86.8450000    -351160.000
    823.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10476.000
 0.000000000D+00 0.000000000D+00 7.853740028D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.305174650D+04-3.455318466D+01
LiCL(cr)          Cubic. Gurvich,1982 pt1 p279 pt2 p313.
 2 tpis82 LI  1.00CL  1.00    0.00    0.00    0.00 1   42.3940000    -408540.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9300.000
-2.180497685D+06 3.971320780D+04-2.918258028D+02 1.160079971D+00-2.482284097D-03
 2.785692272D-06-1.280897066D-09                -2.302427379D+05 1.533139994D+03
    500.000    883.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9300.000
-3.595609330D+04 0.000000000D+00 5.480770500D+00 2.332209108D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.099411730D+04-2.499631307D+01
LiCL(L)           Liquid. Gurvich,1982 pt1 p279 pt2 p313.
 1 tpis82 LI  1.00CL  1.00    0.00    0.00    0.00 2   42.3940000    -408540.000
    883.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9300.000
 0.000000000D+00 0.000000000D+00 7.601169522D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.954114490D+04-3.460716245D+01
LiF(cr)           Cubic. Gurvich,1982 pt1 p273 pt2 p309.
 2 tpis82 LI  1.00F   1.00    0.00    0.00    0.00 1   25.9394032    -618300.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6473.000
 9.636751230D+05-1.777983613D+04 1.305502564D+02-4.624287950D-01 9.558363610D-04
-1.037162482D-06 4.637142460D-10                 5.186488570D+03-6.901111630D+02
    500.000   1122.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6473.000
-7.420484740D+04 0.000000000D+00 5.359396170D+00 1.623955670D-03 2.090115068D-07
 0.000000000D+00 0.000000000D+00                -7.628479220D+04-2.715764184D+01
LiF(L)            Liquid. Gurvich,1982 pt1 p273 pt2 p309.
 1 tpis82 LI  1.00F   1.00    0.00    0.00    0.00 2   25.9394032    -618300.000
   1122.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6473.000
 0.000000000D+00 0.000000000D+00 7.673332524D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.443734250D+04-3.852218670D+01
LiH(cr)           Cubic. Gurvich,1982 pt1 p263 pt2 p300.
 1 tpis82 LI  1.00H   1.00    0.00    0.00    0.00 1    7.9489400     -90650.000
    200.000    965.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          3883.000
-7.983399540D+03-4.135167420D+02 3.842672410D+00 3.568427660D-03 3.560726720D-07
 9.299007330D-10-5.466520940D-13                -9.882374510D+03-2.193513588D+01
LiH(L)            Liquid. Gurvich,1982 pt1 p263 pt2 p300.
 1 tpis82 LI  1.00H   1.00    0.00    0.00    0.00 2    7.9489400     -90650.000
    965.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          3883.000
 0.000000000D+00 0.000000000D+00 6.614941831D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.089088820D+04-3.406734782D+01
LiI(cr)           Cubic. Gurvich,1982 pt1 p287 pt2 p321.
 2 tpis82 LI  1.00I   1.00    0.00    0.00    0.00 1  133.8454700    -273200.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11360.000
-6.958662980D+04 4.035715450D+02 7.056546540D+00-1.824255625D-02 6.907245220D-05
-9.841303530D-08 5.297565590D-11                -3.712485890D+04-2.568066591D+01
    500.000    742.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11360.000
 0.000000000D+00 0.000000000D+00 5.248298340D+00 2.986457552D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.455573620D+04-2.036433073D+01
LiI(L)            Liquid. Gurvich,1982 pt1 p287 pt2 p321.
 1 tpis82 LI  1.00I   1.00    0.00    0.00    0.00 2  133.8454700    -273200.000
    742.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11360.000
 0.000000000D+00 0.000000000D+00 7.601169522D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.371867140D+04-3.132631144D+01
LiNO2(II)         Crystal. Gurvich,1982 pt1 p292 pt2 p326.
 1 tpis82 LI  1.00N   1.00O   2.00    0.00    0.00 1   52.9465000    -368300.000
    298.150    369.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12100.000
 0.000000000D+00 0.000000000D+00-1.026999787D+00 2.885846550D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.527251980D+04 7.831186054D+00
LiNO2(I)          Hexagonal. Gurvich,1982 pt1 p292 pt2 p326.
 1 tpis82 LI  1.00N   1.00O   2.00    0.00    0.00 2   52.9465000    -368300.000
    369.000    495.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12100.000
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.703274180D+04-4.390844045D+01
LiNO2(L)          Liquid. Gurvich,1982 pt1 p292 pt2 p326.
 1 tpis82 LI  1.00N   1.00O   2.00    0.00    0.00 3   52.9465000    -368300.000
    495.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12100.000
 0.000000000D+00 0.000000000D+00 1.082445027D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.652158720D+04-4.913541343D+01
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LiNO3(cr)          Hexagonal. Gurvich,1982 pt1 p294 pt2 p328.
 1 tpis82 LI  1.00N   1.00O   3.00     0.00     0.00 1   68.9459000     -482700.000
    298.150    526.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12800.000
 0.000000000D+00 0.000000000D+00 1.052906305D+01-9.448181552D-03 3.365959028D-05
 0.000000000D+00 0.000000000D+00                 -6.107180100D+04-4.616118415D+01
LiNO3(L)           Liquid. Gurvich,1982 pt1 p294 pt2 p328.
 1 tpis82 LI  1.00N   1.00O   3.00     0.00     0.00 2   68.9459000     -482700.000
    525.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12800.000
 0.000000000D+00 0.000000000D+00 1.792047878D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.162709200D+04-8.706763908D+01
LiOH(cr)           Tetragonal. Gurvich,1996b.
 1 g 9/99 LI  1.00O   1.00H   1.00     0.00     0.00 1   23.9483400     -487500.000
    200.000    746.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7414.000
-1.219596094D+06 2.088315832D+04-1.463475951D+02 5.611592820D-01-1.084380003D-03
 1.071790003D-06-4.218924790D-10                 -1.553535026D+05 7.744131680D+02
LiOH(L)            Liquid. Gurvich,1996b.
 1 g 9/99 LI  1.00O   1.00H   1.00     0.00     0.00 2   23.9483400     -487500.000
    746.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7414.000
 0.000000000D+00 0.000000000D+00 1.049971676D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.050280710D+04-5.407387960D+01
Li2CO3(cr)         Monoclinic. Gurvich,1982 pt1 p297 pt2 p330.
 2 tpis82 LI  2.00C   1.00O   3.00     0.00     0.00 1   73.8909000    -1214100.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15180.000
 1.989594337D+07-3.631706770D+05 2.691242782D+03-1.033109020D+01 2.201400812D-02
-2.454585112D-05 1.122641035D-08                 1.495415902D+06-1.413251128D+04
    500.000   1005.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15180.000
-5.276502280D+04 0.000000000D+00 7.025051540D+00 1.809479379D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.490977245D+05-3.487871400D+01
Li2CO3(L)          Liquid. Gurvich,1982 pt1 p297 pt2 p330.
 1 tpis82 LI  2.00C   1.00O   3.00     0.00     0.00 2   73.8909000    -1214100.000
   1005.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15180.000
 0.000000000D+00 0.000000000D+00 2.225025888D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.502292112D+05-1.169607936D+02
Li2O(cr)           Cubic. Gurvich,1982 pt1 p257 pt2 p295.
 2 tpis82 LI  2.00O   1.00     0.00     0.00     0.00 1   29.8814000     -597880.000
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7251.000
 3.028110639D+05-4.262752720D+03 1.838105970D+01 8.164277890D-03-6.056855750D-05
 8.533995130D-08-3.737236310D-11                 -5.206402060D+04-1.132207799D+02
    800.000   1726.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7251.000
-5.016824310D+06 2.420062743D+04-4.101266390D+01 5.324367340D-02-2.998210001D-05
 1.063865942D-08-1.399118443D-12                 -2.158188563D+05 2.784406390D+02
Li2O(L)            Liquid. Gurvich,1982 pt1 p257 pt2 p295.
 1 tpis82 LI  2.00O   1.00     0.00     0.00     0.00 2   29.8814000     -597880.000
   1726.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7251.000
 0.000000000D+00 0.000000000D+00 1.250825364D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.338860760D+04-6.881025076D+01
Li2O2(cr)          Hexagonal. Gurvich,1982 pt1 p261 pt2 p298.
 1 tpis82 LI  2.00O   2.00     0.00     0.00     0.00 1   45.8808000     -632500.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10500.000
 0.000000000D+00 0.000000000D+00 6.874488094D+00 7.197297255D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.844135590D+04-3.433817812D+01
Li2SO4(a)          Alpha. Gurvich,1982 pt1 p291 pt2 p325.
 2 tpis82 LI  2.00S   1.00O   4.00     0.00     0.00 1  109.9446000    -1436000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18631.000
 2.307314336D+07-4.440850530D+05 3.473570360D+03-1.406997202D+01 3.151077609D-02
-3.672532150D-05 1.742494307D-08                 1.810572013D+06-1.805254507D+04
    500.000    848.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18631.000
 1.379684430D+06 0.000000000D+00-7.865353280D+01 4.280849920D-01-6.782300830D-04
 3.795553140D-07 0.000000000D+00                 -1.584238676D+05 3.687429570D+02
Li2SO4(b)          Beta. Gurvich,1982 pt1 p291 pt2 p325.
 1 tpis82 LI  2.00S   1.00O   4.00     0.00     0.00 2  109.9446000    -1436000.000
    848.000   1131.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18631.000
 0.000000000D+00 0.000000000D+00 2.621922398D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.809832398D+05-1.396630415D+02
Li2SO4(L)          Liquid. Gurvich,1982 pt1 p291 pt2 p325.
 1 tpis82 LI  2.00S   1.00O   4.00     0.00     0.00 3  109.9446000    -1436000.000
   1131.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18631.000
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.780963589D+05-1.276811017D+02
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Li3ALF6(IV)        Rhombic. Gurvich,1982 pt1 p301 pt2 p334.
 2 tpis82 LI  3.00AL  1.00F   6.00    0.00    0.00 1  161.7949572   -3389600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        32150.000
-9.493305210D+05 1.726015181D+04-1.388395633D+02 7.441178510D-01-1.715868367D-03
 2.058073373D-06-9.983283300D-10                -4.893133340D+05 7.043980840D+02
    500.000    788.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        32150.000
-3.361898910D+05 0.000000000D+00 2.259884943D+01 2.065859808D-02-6.977943650D-06
 0.000000000D+00 0.000000000D+00                -4.163946960D+05-1.138999049D+02
Li3ALF6(III)       Tetragonal. Gurvich,1982 pt1 p301 pt2 p334.
 1 tpis82 LI  3.00AL  1.00F   6.00    0.00    0.00 2  161.7949572   -3389600.000
    788.000    873.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        32150.000
 0.000000000D+00 0.000000000D+00 3.427742585D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.195341580D+05-1.769490331D+02
Li3ALF6(II)        Cubic. Gurvich,1982 pt1 p301 pt2 p334.
 1 tpis82 LI  3.00AL  1.00F   6.00    0.00    0.00 3  161.7949572   -3389600.000
    873.000    978.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        32150.000
 0.000000000D+00 0.000000000D+00 3.548014255D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.202233150D+05-1.846804483D+02
Li3ALF6(I)         Crystal. Gurvich,1982 pt1 p301 pt2 p334.
 1 tpis82 LI  3.00AL  1.00F   6.00    0.00    0.00 4  161.7949572   -3389600.000
    978.000   1058.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        32150.000
 0.000000000D+00 0.000000000D+00 3.343552416D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.172975860D+05-1.696552845D+02
Li3ALF6(L)         Liquid. Gurvich,1982 pt1 p301 pt2 p334.
 1 tpis82 LI  3.00AL  1.00F   6.00    0.00    0.00 5  161.7949572   -3389600.000
   1058.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        32150.000
 0.000000000D+00 0.000000000D+00 4.642486448D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.204684280D+05-2.501224871D+02
Li3N(cr)           Chase,1998 p1526.
 2 j 3/78 LI  3.00N   1.00    0.00    0.00    0.00 1   34.8297000    -164557.000
    200.000    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11213.120
 1.373485590D+06-2.379184204D+04 1.591917968D+02-4.823554940D-01 8.557283860D-04
-7.626448860D-07 2.741510774D-10                8.816502990D+04-8.595793090D+02
    700.000   1300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11213.120
-1.241718958D+08 7.830020910D+05-2.032330783D+03 2.815135927D+00-2.148359487D-03
 8.689521850D-07-1.452735248D-10                -4.390747670D+06 1.278810396D+04
Mg(cr)             Hexagonal. Ref-Elm. Alcock,1993.
 2 srd 93 MG  1.00    0.00    0.00    0.00    0.00 1   24.3050000          0.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4979.161
-5.412225134D+03 0.000000000D+00 1.458173723D+00 1.330204666D-02-4.098858502D-05
 4.754339101D-08 0.000000000D+00                -7.759472010D+02-6.989702348D+00
    298.150    923.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4979.161
-2.860060304D+04 0.000000000D+00 3.398877384D+00-7.243962663D-04 1.405254188D-06
 0.000000000D+00 0.000000000D+00                -1.089519906D+03-1.545973664D+01
Mg(L)              Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 MG  1.00    0.00    0.00    0.00    0.00 2   24.3050000          0.000
    923.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4979.161
 0.000000000D+00 0.000000000D+00 4.125318269D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.589919480D+02-1.937828582D+01
MgAL2O4(cr)        Crystal. Chase,1998 pp147-9.
 2 j12/79 MG  1.00AL  2.00O   4.00    0.00    0.00 1  142.2656760   -2299110.000
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        64479.624
 9.746254450D+05-1.525021312D+04 8.302860630D+01-1.382241614D-01 1.657566530D-04
-9.668302460D-08 2.170561037D-11                -2.062543046D+05-4.734083400D+02
    800.000   2408.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        64479.624
-7.339625410D+05 1.248275880D+03 1.548493786D+01 6.232746800D-03-9.669121680D-07
 2.487422341D-10-2.603898110D-14                -2.909147610D+05-7.914855130D+01
MgAL2O4(L)         Liquid. Chase,1998 pp147-9.
 1 j12/79 MG  1.00AL  2.00O   4.00    0.00    0.00 2  142.2656760   -2299110.000
   2408.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        64479.624
 0.000000000D+00 0.000000000D+00 2.641887495D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.688320250D+05-1.419843893D+02
MgBr2(cr)          Hexagonal. Gurvich,1996a pt1 p418 pt2 p332.
 1 tpis96 MG  1.00BR  2.00    0.00    0.00    0.00 1  184.1130000    -526000.000
    298.150    984.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15500.499
-6.657036915D+04 0.000000000D+00 9.124771033D+00 1.443260036D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.627087500D+04-3.872222733D+01
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MgBr2(L)          Liquid. Gurvich,1996a pt1 p418 pt2 p332.
 1 tpis96 MG  1.00BR  2.00    0.00    0.00    0.00 2  184.1130000    -526000.000
    984.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15500.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.363378060D+04-5.246637684D+01
MgCO3(cr)         Hexagonal. Gurvich,1996a pt1 p429 pt2 p341.
 2 tpis96 MG  1.00C   1.00O   3.00    0.00    0.00 1   84.3139000   -1096000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11630.499
-5.649471920D+06 1.059809340D+05-8.095953810D+02 3.267992680D+00-7.111639940D-03
 8.088247340D-06-3.758639920D-09                -6.098528470D+05 4.221968000D+03
    500.000   1263.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11630.499
-1.743337852D+05 0.000000000D+00 8.820122894D+00 7.696184141D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.353742560D+05-4.570039759D+01
MgCO3(L)          Liquid. Gurvich,1996a pt1 p429 pt2 p341.
 1 tpis96 MG  1.00C   1.00O   3.00    0.00    0.00 3   84.3139000   -1096000.000
   1263.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11630.499
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.336474914D+05-9.615384273D+01
MgCL2(cr)         Hexagonal. Gurvich,1996a pt1 p413 pt2 p329.
 2 tpis96 MG  1.00CL  2.00    0.00    0.00    0.00 1   95.2110000    -644300.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13770.499
 3.151271437D+05-4.986561670D+03 3.407490430D+01-6.013327030D-02 7.256223640D-05
-2.984411528D-08-5.064069590D-12                -5.608909370D+04-1.833415814D+02
    500.000    987.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13770.499
-7.745495525D+04 0.000000000D+00 9.099153167D+00 1.199709905D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.051706960D+04-4.185795845D+01
MgCL2(L)          Liquid. Gurvich,1996a pt1 p413 pt2 p329.
 1 tpis96 MG  1.00CL  2.00    0.00    0.00    0.00 3   95.2110000    -644300.000
    987.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13770.499
 7.120082843D+05 0.000000000D+00 1.060122605D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.543168500D+04-4.537295861D+01
MgF2(cr)          Tetragonal. Gurvich,1996a pt1 p410 pt2 p326.
 2 tpis96 MG  1.00F   2.00    0.00    0.00    0.00 1   62.3018064    -1124200.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9920.499
-8.758857470D+06 1.630690293D+05-1.234784473D+03 4.913114430D+00-1.064398199D-02
 1.204196054D-05-5.572295890D-09                -8.710379520D+05 6.452721700D+03
    500.000   1536.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9920.499
-1.863609521D+05 0.000000000D+00 9.358338615D+00 4.871002621D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.386463039D+05-4.763420955D+01
MgF2(L)           Liquid. Gurvich,1996a pt1 p410 pt2 p326.
 1 tpis96 MG  1.00F   2.00    0.00    0.00    0.00 3   62.3018064    -1124200.000
   1536.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9920.499
 0.000000000D+00 0.000000000D+00 1.140175428D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.340531621D+05-5.725828106D+01
MgH2(b)           Beta,tetragonal. Gurvich,1996a pt1 p402 pt2 p321.
 1 tpis96 MG  1.00H   2.00    0.00    0.00    0.00 1   26.3208800     -75700.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5310.000
 4.034912200D+06-6.115400800D+04 3.537084270D+02-9.554057160D-01 1.260522797D-03
-6.389211330D-07 0.000000000D+00                2.799920215D+05-1.959491159D+03
MgH2(L)           Liquid. Gurvich,1996a pt1 p402 pt2 p321.
 1 tpis96 MG  1.00H   2.00    0.00    0.00    0.00 2   26.3208800     -75700.000
    600.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5310.000
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.135051728D+04-4.777194561D+01
MgI2(cr)          Hexagonal. Gurvich,1996a pt1 p422 pt2 p335.
 1 tpis96 MG  1.00I   2.00    0.00    0.00    0.00 1  278.1139400    -370000.000
    298.150    906.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17000.499
 0.000000000D+00 0.000000000D+00 8.291528905D+00 2.232723275D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.707187430D+04-3.179107057D+01
MgI2(L)           Liquid. Gurvich,1996a pt1 p422 pt2 p335.
 1 tpis96 MG  1.00I   2.00    0.00    0.00    0.00 2  278.1139400    -370000.000
    906.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17000.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.641294920D+04-5.175282479D+01
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MgO(cr)           Cubic Gurvich,1996a pt1 p397 pt2 p317.
 2 tpis96 MG  1.00O   1.00    0.00    0.00    0.00 1   40.3044000    -601600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5160.499
-8.980784570D+05 1.771245421D+04-1.449325747D+02 6.397591100D-01-1.458346800D-03
 1.715467374D-06-8.183482370D-10                 -1.516290864D+05 7.439009690D+02
    500.000   3100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5160.499
-1.169521716D+05 0.000000000D+00 5.510366817D+00 1.085932905D-03-4.866191754D-07
 1.253230798D-10 0.000000000D+00                 -7.443482720D+04-2.911564935D+01
MgO(L)            Liquid Gurvich,1996a pt1 p397 pt2 p317.
 1 tpis96 MG  1.00O   1.00    0.00    0.00    0.00 3   40.3044000    -601600.000
   3100.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5160.499
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.609370840D+04-6.076894048D+01
Mg(OH)2(cr)       Hexagonal. Gurvich,1996a pt1 p405 pt2 p323.
 2 tpis96 MG  1.00O   2.00H   2.00    0.00    0.00 1   58.3196800    -924350.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11410.000
-6.401451840D+05 8.358139990D+03-3.971145400D+01 1.231927219D-01-9.647800650D-05
 0.000000000D+00 0.000000000D+00                 -1.537246903D+05 2.258495398D+02
    500.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11410.000
-5.543828430D+06 3.700868610D+04-9.088623340D+01 1.431689186D-01-9.513965240D-05
 2.532586546D-08 0.000000000D+00                 -3.189450890D+05 5.801638270D+02
Mg(OH)2(L)        Liquid. Gurvich,1996a pt1 p405 pt2 p323.
 1 tpis96 MG  1.00O   2.00H   2.00    0.00    0.00 2   58.3196800    -924350.000
   1100.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11410.000
-3.037581289D+05 0.000000000D+00 1.203462381D+01 2.202655358D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.158775486D+05-6.333852645D+01
MgS(cr)           Cubic. Gurvich,1996a pt1 p424 pt2 p337.
 2 tpis96 MG  1.00S   1.00    0.00    0.00    0.00 1   56.3700000    -348000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8330.499
 1.862529340D+06-3.536941040D+04 2.721839670D+02-1.042907730D+00 2.246733361D-03
-2.528313530D-06 1.164923631D-09                 1.157121957D+05-1.421776433D+03
    500.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8330.499
-2.774667419D+04 0.000000000D+00 5.477652922D+00 1.053219011D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.362757840D+04-2.562621459D+01
MgS(L)            Liquid. Gurvich,1996a pt1 p424 pt2 p337.
 1 tpis96 MG  1.00S   1.00    0.00    0.00    0.00 3   56.3700000    -348000.000
   2500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8330.499
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.919942750D+04-4.015043492D+01
MgSO4(II)         CrII,rhombic. Gurvich,1996a pt1 p426 pt2 p339.
 2 tpis96 MG  1.00S   1.00O   4.00    0.00    0.00 1  120.3676000   -1288800.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
 7.038799190D+06-1.283866938D+05 9.464955820D+02-3.562117130D+00 7.535844540D-03
-8.351428640D-06 3.800035070D-09                 4.243566150D+05-4.979377480D+03
    500.000   1283.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
-1.403690656D+05 0.000000000D+00 1.024474082D+01 1.053279147D-02-2.384385851D-06
 0.000000000D+00 0.000000000D+00                 -1.589785092D+05-5.117735953D+01
MgSO4(I)          CrI,rhombic. Gurvich,1996a pt1 p426 pt2 p339.
 1 tpis96 MG  1.00S   1.00O   4.00    0.00    0.00 3  120.3676000   -1288800.000
   1283.000   1410.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.622917080D+05-9.940197517D+01
MgSO4(L)          Liquid. Gurvich,1996a pt1 p426 pt2 p339.
 1 tpis96 MG  1.00S   1.00O   4.00    0.00    0.00 4  120.3676000   -1288800.000
   1410.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.605357417D+05-9.815660894D+01
MgSiO3(I)         Chase,1998 pp1540-2.
 1 j12/67 MG  1.00SI  1.00O   3.00    0.00    0.00 1  100.3887000   -1548916.800
    200.000    903.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12112.680
 6.634624630D+05-1.098828549D+04 6.661582640D+01-1.408979556D-01 2.056144180D-04
-1.506280668D-07 4.456006950D-11                 -1.365977193D+05-3.704100780D+02
MgSiO3(II)        Chase,1998 pp1540-2.
 1 j12/67 MG  1.00SI  1.00O   3.00    0.00    0.00 2  100.3887000   -1548916.800
    903.000   1258.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12112.680
 0.000000000D+00 0.000000000D+00 1.447351774D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.916168640D+05-7.665690420D+01
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MgSiO3(III)        Chase,1998 pp1540-2.
 1 j12/67 MG  1.00SI  1.00O   3.00     0.00     0.00 3  100.3887000   -1548916.800
   1258.000   1850.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12112.680
 0.000000000D+00 0.000000000D+00 1.472512607D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.917371327D+05-7.829669776D+01
MgSiO3(L)          Chase,1998 pp1540-2.
 1 j12/67 MG  1.00SI  1.00O   3.00     0.00     0.00 4  100.3887000   -1548916.800
   1850.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12112.680
 0.000000000D+00 0.000000000D+00 1.761258330D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.880210286D+05-9.512270574D+01
MgTiO3(cr)         Chase,1998 pp1543-5.
 2 j 6/67 MG  1.00TI  1.00O   3.00     0.00     0.00 1  120.1702000   -1572556.400
    200.000    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13556.160
 7.429774000D+05-1.292212821D+04 8.410507170D+01-2.098263307D-01 3.615281930D-04
-3.238214780D-07 1.180955355D-10                -1.313766506D+05-4.602729640D+02
    700.000   1953.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13556.160
 1.601922450D+05-2.633226069D+03 1.883800780D+01-1.678968165D-03 1.139243183D-06
-2.244954628D-10 2.663226969D-14                -1.791724552D+05-1.059181291D+02
MgTiO3(L)          Chase,1998 pp1543-5.
 1 j 6/67 MG  1.00TI  1.00O   3.00     0.00     0.00 2  120.1702000   -1572556.400
   1953.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13556.160
 0.000000000D+00 0.000000000D+00 1.962544997D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.909134805D+05-1.065587855D+02
MgTi2O5(cr)        Todd,1952. Chase,1998 pp1550-1552 6/67.
 2 g11/00 MG  1.00TI  2.00O   5.00     0.00     0.00 1  200.0360000   -2508218.800
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22438.792
 1.244806767D+06-2.122898938D+04 1.352816814D+02-3.207171960D-01 5.056737150D-04
-4.075110600D-07 1.330675670D-10                -2.063427950D+05-7.421883210D+02
    800.000   1963.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22438.792
 1.206826103D+06-7.504042080D+03 3.472504430D+01-9.398048060D-03 7.725115420D-06
-2.268307646D-09 2.728749772D-13                -2.651238294D+05-1.981547532D+02
MgTi2O5(L)         Todd,1952. Chase,1998 pp1550-1552 6/67.
 1 g11/00 MG  1.00TI  2.00O   5.00     0.00     0.00 2  200.0360000   -2508218.800
   1963.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22438.792
 0.000000000D+00 0.000000000D+00 3.140071995D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.039563022D+05-1.685813857D+02
Mg2SiO4(cr)        Chase,1998 pp1556-8 12/67.
 2 g11/00 MG  2.00SI  1.00O   4.00     0.00     0.00 1  140.6931000   -2177078.400
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17279.920
 9.212035030D+05-1.508156349D+04 9.085102220D+01-1.898897815D-01 2.890690717D-04
-2.266693109D-07 7.230688250D-11                -1.936097830D+05-5.059650070D+02
    800.000   2171.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17279.920
 3.714548590D+06-2.041518891D+04 5.788009140D+01-3.629874490D-02 2.183358474D-05
-6.504809080D-09 7.908133680D-13                -1.494870518D+05-3.576608370D+02
Mg2SiO4(L)         Chase,1998 pp1556-8 12/67
 1 g11/00 MG  2.00SI  1.00O   4.00     0.00     0.00 2  140.6931000   -2177078.400
   2170.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17279.920
 0.000000000D+00 0.000000000D+00 2.465761662D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.669357683D+05-1.346103798D+02
Mg2TiO4(cr)        Chase,1998 pp1559-61 6/67.
 2 g11/00 MG  2.00TI  1.00O   4.00     0.00     0.00 1  160.4746000   -2164354.400
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18836.368
 9.956749990D+05-1.724659186D+04 1.091877188D+02-2.478088109D-01 3.830393010D-04
-3.022256428D-07 9.684735620D-11                -1.830794683D+05-6.011710070D+02
    800.000   2013.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18836.368
 3.251168130D+05-3.023737890D+03 2.335313762D+01-5.057540210D-04 2.750958409D-06
-9.172292550D-10 1.089453371D-13                -2.490728250D+05-1.278129303D+02
Mg2TiO4(L)         Chase,1998 pp1559-61 6/67.
 1 g11/00 MG  2.00TI  1.00O   4.00     0.00     0.00 2  160.4746000   -2164354.400
   2013.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18836.368
 0.000000000D+00 0.000000000D+00 2.747562995D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.615257868D+05-1.474539637D+02
Mg3N2(cr)          Cubic. Gurvich,1996a pt1 p427 pt2 p340.
 1 tpis96 MG  3.00N   2.00     0.00     0.00     0.00 1  100.9284000    -461300.000
    298.150   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10500.499
-3.313123684D+05 0.000000000D+00 1.448912804D+01 1.035659347D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.095851350D+04-7.450243529D+01
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Mn(a)              Alpha. Ref-Elm. Chase,1998 pp1571-4.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 1   54.9380490          0.000
    200.000    980.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4994.000
-1.984724642D+04 1.808814126D+02 1.038289801D+00 8.813332010D-03-1.298045968D-05
 1.118858744D-08-3.673641300D-12                -1.704143022D+03-3.713160980D+00
Mn(b)              Beta. Ref-Elm. Chase,1998 pp1571-4.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 2   54.9380490          0.000
    980.000   1361.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4994.000
-2.033299729D+08 8.595009270D+05-1.444429639D+03 1.217025958D+00-5.092264580D-04
 8.499457640D-08 0.000000000D+00                -5.153128480D+06 9.753553620D+03
Mn(c)              Gamma. Ref-Elm. Chase,1998 pp1571-4.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 3   54.9380490          0.000
   1361.000   1412.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4994.000
-5.539443490D+06 0.000000000D+00 1.249195042D+01-3.172888290D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.319440868D+04-7.701110710D+01
Mn(d)              Delta. Ref-Elm. Chase,1998 pp1571-4.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 4   54.9380490          0.000
   1412.000   1519.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4994.000
-4.256613510D+06 0.000000000D+00 1.001289188D+01-1.726727732D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.000110470D+04-6.059129950D+01
Mn(L)              Liquid. Ref-Elm. Chase,1998 pp1571-4.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 5   54.9380490          0.000
   1519.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4994.000
 0.000000000D+00 0.000000000D+00 5.535383324D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.393783130D+02-2.853570386D+01
Mo(cr)             Crystal. Ref-Elm. Chase,1998 pp1577-80.
 3 j 3/78 MO  1.00    0.00    0.00    0.00    0.00 1   95.9400000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4585.000
-4.961689320D+04 4.280941190D+02 7.671984690D-01 5.731518250D-03-6.381641180D-06
 3.708192420D-09-7.917347080D-13                -3.039584622D+03-1.230467690D+00
   1000.000   2200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4585.000
-3.617592720D+06 1.474639904D+04-2.136672658D+01 2.118577261D-02-9.789741690D-06
 2.496130112D-09-2.422303123D-13                -8.977896080D+04 1.507160275D+02
   2200.000   2896.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4585.000
 4.759909590D+09-5.321527320D+06-8.747403120D+02 3.794789480D+00-2.131568725D-03
 4.974075900D-07-4.325425090D-11                 4.096569650D+07 1.130483988D+02
Mo(L)              Liquid. Ref-Elm. Chase,1998 pp1577-80.
 1 j 3/78 MO  1.00    0.00    0.00    0.00    0.00 2   95.9400000          0.000
   2896.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4585.000
 0.000000000D+00 0.000000000D+00 4.528949992D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.022300696D+03-2.280790783D+01
MoO2(cr)           Monoclinic. Gurvich,1982 pt1 p27 pt2 p32.
 2 tpis82 MO  1.00O   2.00    0.00    0.00    0.00 1  127.9388000    -589300.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8328.000
-6.526622370D+06 1.230156278D+05-9.443937510D+02 3.807393330D+00-8.319729080D-03
 9.477106540D-06-4.408972390D-09                -6.244588120D+05 4.921849140D+03
    500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8328.000
-2.051418601D+05 0.000000000D+00 8.963295880D+00-1.128973209D-04 1.146693959D-06
 0.000000000D+00 0.000000000D+00                -7.424162440D+04-4.664669130D+01
MoO3(cr)           Rhombic. Gurvich,1982 pt1 p30 pt2 p34.
 2 tpis82 MO  1.00O   3.00    0.00    0.00    0.00 1  143.9382000    -744600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12590.000
 9.061545810D+06-1.658675979D+05 1.230236799D+03-4.691503730D+00 9.965828580D-03
-1.109194136D-05 5.065628490D-09                 6.590937470D+05-6.461598540D+03
    500.000   1075.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12590.000
-9.462974968D+04 0.000000000D+00 8.841771794D+00 4.197842086D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.269445280D+04-4.282025959D+01
MoO3(L)            Liquid. Gurvich,1982 pt1 p30 pt2 p34.
 1 tpis82 MO  1.00O   3.00    0.00    0.00    0.00 3  143.9382000    -744600.000
   1075.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12590.000
 0.000000000D+00 0.000000000D+00 1.527450205D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.123881420D+04-7.771899557D+01
NH4CL(II)          Chase,1998 p765.
 1 j 9/65 N   1.00H   4.00CL  1.00    0.00    0.00 1   53.4914600    -314553.000
    298.150    457.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22698.000
 1.593389657D+05 0.000000000D+00-5.965854940D+00 6.494193170D-02-5.391456890D-05
 0.000000000D+00 0.000000000D+00                -3.792881500D+04 2.933013040D+01
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NH4CL(III)          Chase,1998 p765.
 2 j 9/65 N   1.00H   4.00CL  1.00    0.00    0.00 2   53.4914600    -314553.000
    457.700   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22698.000
-1.641820157D+07 1.639262758D+05-6.654529630D+02 1.447086973D+00-1.698254160D-03
 1.056255415D-06-2.697574651D-10                -8.787975900D+05 3.897936900D+03
   1000.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22698.000
 8.409592660D+08-3.426760780D+06 5.548091470D+03-4.435674300D+00 1.772486202D-03
-2.817160120D-07 0.000000000D+00                 2.063363145D+07-3.765976360D+04
NH4F(cr)            Hexagonal. Gurvich,1989 pt1 p388 pt2 p324.
 2 tpis89 N   1.00H   4.00F   1.00    0.00    0.00 1   37.0368632    -467560.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11108.000
-2.975636383D+06 7.208754230D+04-7.346289470D+02 4.075299810D+00-1.264044498D-02
 2.111837237D-05-1.479873524D-08                -3.621184440D+05 3.608760970D+03
    298.150    511.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11108.000
 0.000000000D+00 0.000000000D+00 1.563531705D+00 2.108482641D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.763754000D+04-6.538862038D+00
NH4F(L)             Liquid. Gurvich,1989 pt1 p388 pt2 p324.
 1 tpis89 N   1.00H   4.00F   1.00    0.00    0.00 2   37.0368632    -467560.000
    511.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11108.000
 0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.951515380D+04-6.780477125D+01
Na(cr)              Cubic. Ref-Elm. Cox,1989 p254.
 1 coda89 NA  1.00    0.00    0.00    0.00    0.00 1   22.9897700          0.000
    200.000    371.0107 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6460.000
-3.584458010D+04 0.000000000D+00 6.479414690D+00-1.898697341D-02 3.352387090D-05
 0.000000000D+00 0.000000000D+00                -1.504319740D+03-2.677783039D+01
Na(L)               Liquid. Ref-Elm. Cox,1989 p254.
 1 coda89 NA  1.00    0.00    0.00    0.00    0.00 2   22.9897700          0.000
    371.010   2300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6460.000
 2.694818670D+04-2.319000780D+02 5.162435690D+00-3.058571990D-03 1.696407999D-06
-1.519633426D-10 1.962859159D-14                 2.842114288D+02-2.225763980D+01
NaALO2(a)           Alpha.Chase,1998 p131.
 1 j 3/63 NA  1.00AL  1.00O   2.00    0.00    0.00 1   81.9701080   -1133190.000
    200.000    740.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23794.000
 4.527204140D+05-7.722924360D+03 5.000166380D+01-1.091293529D-01 1.762084005D-04
-1.452865027D-07 4.918123650D-11                -1.021205450D+05-2.738871707D+02
NaALO2(b)           Beta. Chase,1998 p131.
 1 j 3/63 NA  1.00AL  1.00O   2.00    0.00    0.00 2   81.9701080   -1133190.000
    740.000   3000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23794.000
 3.197980170D+06-1.525937524D+04 3.932924030D+01-2.623291355D-02 1.465112353D-05
-3.740532770D-09 3.560249390D-13                -4.988553210D+04-2.434131708D+02
NaBO2(cr)           Hexagonal. Gurvich,1982 pt1 p357 pt2 p391.
 2 tpis82 NA  1.00B   1.00O   2.00    0.00    0.00 1   65.7995700    -976500.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11632.000
-1.074702306D+05 2.343688910D+03-1.964636192D+01 1.319434021D-01-2.997058540D-04
 3.640103610D-07-1.796104124D-10                -1.291527393D+05 9.915788280D+01
    500.000   1239.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11632.000
-5.597627870D+04 0.000000000D+00 5.491743560D+00 1.171509302D-02-4.773472260D-06
 0.000000000D+00 0.000000000D+00                -1.197489098D+05-2.604168849D+01
NaBO2(L)            Liquid. Gurvich,1982 pt1 p357 pt2 p391.
 1 tpis82 NA  1.00B   1.00O   2.00    0.00    0.00 2   65.7995700    -976500.000
   1239.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11632.000
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.245121293D+05-9.701235601D+01
NaBr(cr)            Cubic. Gurvich,1982 pt1 p340 pt2 p378.
 2 tpis82 NA  1.00BR  1.00    0.00    0.00    0.00 1  102.8937700    -361160.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11590.000
 3.210289070D+06-5.986721400D+04 4.572531830D+02-1.768432397D+00 3.814169490D-03
-4.295102010D-06 1.980139146D-09                 2.245558598D+05-2.385763453D+03
    500.000   1020.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11590.000
 1.593247644D+04 0.000000000D+00 5.272913580D+00 2.440774360D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.506450850D+04-2.022580453D+01
NaBr(L)             Liquid. Gurvich,1982 pt1 p340 pt2 p378.
 1 tpis82 NA  1.00BR  1.00    0.00    0.00    0.00 2  102.8937700    -361160.000
   1020.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11590.000
 0.000000000D+00 0.000000000D+00 8.178473536D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.361938300D+04-3.477943790D+01
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NaCN(II)          Lambda trans@288.5K. Chase,1998(3/66) pp631-3. Messer,1941.
 6 g 8/01 NA  1.00C   1.00N   1.00     0.00     0.00 1   49.0071700      -90709.000
    197.700    245.9007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
 4.995073610D+08-1.007656780D+07 7.458386410D+04-2.134406974D+02-6.965856220D-02
 1.540182072D-03-2.204709373D-06                 4.493712560D+07-3.984423000D+05
    245.900    273.1007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
-4.546907220D+08 4.339535660D+06 5.476070770D+02-1.324240852D+02 5.045446840D-01
-5.791737950D-04 0.000000000D+00                -2.385188911D+07 3.106410058D+04
    273.100    284.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
-4.415096320D+08 0.000000000D+00 3.452631670D+04-1.661761169D+02 2.250608921D-01
 0.000000000D+00 0.000000000D+00                -6.388306670D+06-1.596447272D+05
    284.200    286.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
 1.647379186D+09 0.000000000D+00-6.100370390D+04 1.429224260D+02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.735057318D+07 3.142435378D+05
    286.300    287.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
 1.607424258D+11 0.000000000D+00-8.629992400D+06 3.290155880D+04-3.355904228D+01
 0.000000000D+00 0.000000000D+00                 1.946284579D+09 4.175641230D+07
    287.700    288.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
-1.494237648D+11 0.000000000D+00 8.652205900D+06-3.521604880D+04 3.968501633D+01
 0.000000000D+00 0.000000000D+00                -1.866195945D+09-4.140143280D+07
NaCN(III)         Lambda trans@288.5K. Chase,1998(3/66) pp631-3. Messer,1941.
 3 g 8/01 NA  1.00C   1.00N   1.00     0.00     0.00 2   49.0071700      -90709.000
    288.500    290.4007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
 0.000000000D+00 0.000000000D+00 5.590153690D+06-4.787600130D+04 1.309325625D+02
-1.114230434D-01 0.000000000D+00                -4.753893060D+08-2.241133349D+07
    290.400    293.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
 0.000000000D+00 0.000000000D+00 1.752406137D+07-1.788423367D+05 6.083847560D+02
-6.898560518D-01 0.000000000D+00                -1.287828620D+09-6.746932890D+07
    293.150    835.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
 0.000000000D+00 0.000000000D+00 8.303074986D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.338528469D+04-3.306050253D+01
NaCN(L)           Chase,1998(3/66) pp631-3. Messer,1941.
 1 g 8/01 NA  1.00C   1.00N   1.00     0.00     0.00 3   49.0071700      -90709.000
    835.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19422.128
 0.000000000D+00 0.000000000D+00 9.561116650D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.337899448D+04-4.025831708D+01
NaCL(cr)          Cubic. Gurvich,1982 pt1 p335 pt2 p374.
 2 tpis82 NA  1.00CL  1.00     0.00     0.00     0.00 1   58.4427700     -411260.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10600.000
 2.725695501D+06-5.160958750D+04 3.984582310D+02-1.547496756D+00 3.352172310D-03
-3.787781590D-06 1.751729541D-09                1.807530763D+05-2.076949046D+03
    500.000   1074.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10600.000
 2.657827371D+03 0.000000000D+00 5.665718690D+00 8.708901490D-04 1.340560030D-06
 0.000000000D+00 0.000000000D+00                -5.119384720D+04-2.390773149D+01
NaCL(L)           Liquid. Gurvich,1982 pt1 p335 pt2 p374.
 1 tpis82 NA  1.00CL  1.00     0.00     0.00     0.00 2   58.4427700     -411260.000
   1074.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10600.000
 0.000000000D+00 0.000000000D+00 8.166446369D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.943459010D+04-3.649536621D+01
NaF(cr)           Cubic. Gurvich,1982 pt1 p330 pt2 p370.
 2 tpis82 NA  1.00F   1.00     0.00     0.00     0.00 1   41.9881732     -576600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8482.000
-6.479380410D+06 1.203694117D+05-9.069923560D+02 3.596486550D+00-7.775987760D-03
 8.784072120D-06-4.059177020D-09                -6.130723750D+05 4.744846560D+03
    500.000   1269.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8482.000
-1.103659993D+05 0.000000000D+00 7.264294880D+00-1.973449856D-03 2.198504269D-06
 0.000000000D+00 0.000000000D+00                -7.181627510D+04-3.536594020D+01
NaF(L)            Liquid. Gurvich,1982 pt1 p330 pt2 p370.
 1 tpis82 NA  1.00F   1.00     0.00     0.00     0.00 2   41.9881732     -576600.000
   1269.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8482.000
 0.000000000D+00 0.000000000D+00 8.431044042D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.918200450D+04-4.115725624D+01
NaH(cr)           Cubic. Gurvich,1982 pt1 p324 pt2 p365.
 2 tpis82 NA  1.00H   1.00     0.00     0.00     0.00 1   23.9977100      -56380.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6259.000
-7.991749220D+05 1.540118135D+04-1.207582590D+02 5.162361030D-01-1.142424910D-03
 1.321529809D-06-6.221705120D-10                -7.637675350D+04 6.264186650D+02
    500.000    911.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6259.000
-5.921209820D+04 0.000000000D+00 3.776579530D+00 4.250132020D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.294394750D+03-1.830678857D+01
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NaH(L)              Liquid. Gurvich,1982 pt1 p324 pt2 p365.
 1 tpis82 NA  1.00H   1.00     0.00     0.00     0.00 2   23.9977100     -56380.000
    911.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6259.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.034013160D+03-3.112842170D+01
NaI(cr)             Cubic. Gurvich,1982 pt1 p343 pt2 p381.
 2 tpis82 NA  1.00I   1.00     0.00     0.00     0.00 1  149.8942400     -289630.000
    200.000     500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12260.000
 3.500848300D+06-6.540492260D+04 5.005676630D+02-1.943541204D+00 4.201134090D-03
-4.738515580D-06 2.187428593D-09                 2.579135069D+05-2.609575154D+03
    500.000     934.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12260.000
 2.799960757D+04 0.000000000D+00 5.047026160D+00 3.029892968D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.637984440D+04-1.764780816D+01
NaI(L)              Liquid. Gurvich,1982 pt1 p343 pt2 p381.
 1 tpis82 NA  1.00I   1.00     0.00     0.00     0.00 2  149.8942400     -289630.000
    934.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12260.000
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.505265490D+04-3.237951568D+01
NaNO2(I)            Rhombic. Gurvich,1982 pt1 p350 pt2 p386.
 2 tpis82 NA  1.00N   1.00O    2.00     0.00     0.00 1   68.9952700     -354600.000
    298.150     400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16500.000
 1.090298767D+06 0.000000000D+00-3.023894373D+01 8.811824148D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.389227900D+04 1.648982675D+02
    400.000     436.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16500.000
 0.000000000D+00 0.000000000D+00 5.419446245D+02-1.998525469D+00 0.000000000D+00
 4.207630035D-06 0.000000000D+00                 -1.254887886D+05-2.521831769D+03
NaNO2(I')           Rhombic. Gurvich,1982 pt1 p350 pt2 p386.
 1 tpis82 NA  1.00N   1.00O    2.00     0.00     0.00 2   68.9952700     -354600.000
    436.700     557.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16500.000
 0.000000000D+00 0.000000000D+00 1.599613206D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.773155280D+04-7.952982535D+01
NaNO2(L)            Liquid. Gurvich,1982 pt1 p350 pt2 p386.
 1 tpis82 NA  1.00N   1.00O    2.00     0.00     0.00 3   68.9952700     -354600.000
    557.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16500.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.372398050D+04-5.120982634D+01
NaNO3(a)            Hexagonal. Gurvich,1982 pt1 p353 pt2 p388.
 2 tpis82 NA  1.00N   1.00O    3.00     0.00     0.00 1   84.9946700     -467700.000
    200.000     500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17230.000
-4.851300240D+07 9.186316330D+05-7.046384650D+03 2.807834358D+01-6.098595830D-02
 6.858389720D-05-3.110743577D-08                 -4.182115940D+06 3.676430560D+04
    500.000     549.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17230.000
 0.000000000D+00 0.000000000D+00 2.680735245D+01-1.753272291D-01 3.165502236D-04
 0.000000000D+00 0.000000000D+00                 -5.811076460D+04-9.741742276D+01
NaNO3(b)            Hexagonal. Gurvich,1982 pt1 p353 pt2 p388.
 1 tpis82 NA  1.00N   1.00O    3.00     0.00     0.00 2   84.9946700     -467700.000
    549.000     579.6007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17230.000
 0.000000000D+00 0.000000000D+00 1.683803375D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.159974430D+04-8.308035085D+01
NaNO3(L)            Liquid. Gurvich,1982 pt1 p353 pt2 p388.
 1 tpis82 NA  1.00N   1.00O    3.00     0.00     0.00 3   84.9946700     -467700.000
    579.600    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17230.000
 0.000000000D+00 0.000000000D+00 1.695830542D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.985936520D+04-8.072256364D+01
NaOH(a)             Alpha. Gurvich,1996b.
 2 g 5/99 NA  1.00O   1.00H    1.00     0.00     0.00 1   39.9971100     -425800.000
    100.000     298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10490.000
 2.008329119D+04-7.714677160D+02 8.694171090D+00 3.850883340D-03-3.610498540D-06
 0.000000000D+00 0.000000000D+00                 -4.948023450D+04-4.524899570D+01
    298.150     514.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10490.000
 1.048215710D+06 0.000000000D+00-9.592892425D+01 6.189564989D-01-1.367212259D-03
 1.067453163D-06 0.000000000D+00                 -3.663541040D+04 4.270051072D+02
NaOH(b)             Beta.  Gurvich,1996b.
 1 g 5/99 NA  1.00O   1.00H    1.00     0.00     0.00 2   39.9971100     -425800.000
    514.000     568.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10490.000
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.442558950D+04-4.799292559D+01
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NaOH(c)            Gamma. Gurvich,1996b.
 1 g 5/99 NA  1.00O   1.00H   1.00     0.00     0.00 3   39.9971100    -425800.000
    568.000    594.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10490.000
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.407054750D+04-5.122288687D+01
NaOH(L)            Liquid. Gurvich,1996b.
 2 g 5/99 NA  1.00O   1.00H   1.00     0.00     0.00 4   39.9971100    -425800.000
    594.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10490.000
 0.000000000D+00 0.000000000D+00 1.077790513D+01-7.111663826D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.343827480D+04-5.228806116D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10490.000
 0.000000000D+00 0.000000000D+00 1.006673875D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.308269160D+04-4.808666421D+01
NaO2(cr)           Cubic. Gurvich,1982 pt1 p319 pt2 p359.Chase,1998 p1646 6/63.
 1 g10/99 NA  1.00O   2.00    0.00     0.00     0.00 1   54.9885700    -261000.000
    223.300    825.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18300.000
 0.000000000D+00 0.000000000D+00 7.541274230D+00 3.803351009D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.380838310D+04-3.016162188D+01
NaO2(L)            Liq. Gurvich,1982 pt1 p319 pt2 p359.Chase,1998 p1646 6/63.
 1 g10/99 NA  1.00O   2.00    0.00     0.00     0.00 2   54.9885700    -261000.000
    825.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18300.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.374934750D+04-5.415977808D+01
Na2CO3(a)          Alpha,monoclinic. Gurvich,1982 pt1 p356 pt2 p390.
 1 tpis82 NA  2.00C   1.00O   3.00     0.00     0.00 1  105.9884400   -1129190.000
    200.000    623.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20750.000
-2.240230091D+06 3.426046630D+04-2.061520520D+02 7.168720430D-01-1.253560327D-03
 1.178136083D-06-4.526962410D-10                 -2.999635262D+05 1.125584713D+03
Na2CO3(b)          Beta,monoclinic. Gurvich,1982 pt1 p356 pt2 p390.
 1 tpis82 NA  2.00C   1.00O   3.00     0.00     0.00 2  105.9884400   -1129190.000
    623.000    752.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20750.000
 0.000000000D+00 0.000000000D+00 7.711578914D+00 1.943638290D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.388766027D+05-3.334178005D+01
Na2CO3(c)          Gamma,hexagonal. Gurvich,1982 pt1 p356 pt2 p390.
 1 tpis82 NA  2.00C   1.00O   3.00     0.00     0.00 3  105.9884400   -1129190.000
    752.000   1131.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20750.000
 0.000000000D+00 0.000000000D+00 4.430327223D+00 1.645316441D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.353130199D+05-9.031669943D+00
Na2CO3(L)          Liquid. Gurvich,1982 pt1 p356 pt2 p390.
 1 tpis82 NA  2.00C   1.00O   3.00     0.00     0.00 4  105.9884400   -1129190.000
   1131.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20750.000
 0.000000000D+00 0.000000000D+00 2.345297558D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.429369053D+05-1.211911225D+02
Na2O(c)            Gamma. Gurvich,1982 pt1 p320 pt2 p360.
 2 tpis82 NA  2.00O   1.00    0.00     0.00     0.00 1   61.9789400    -414570.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12400.000
 1.662637910D+06-3.189091340D+04 2.474349303D+02-9.313593580D-01 2.006501256D-03
-2.253952071D-06 1.037067374D-09                 9.127774380D+04-1.292003778D+03
    500.000   1023.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12400.000
 2.551096288D+05-2.539111311D+03 1.659817003D+01-1.233767744D-02 1.540713549D-05
-8.084697830D-09 1.747972425D-12                 -3.906526610D+04-8.958024740D+01
Na2O(b)            Beta. Gurvich,1982 pt1 p320 pt2 p360.
 1 tpis82 NA  2.00O   1.00    0.00     0.00     0.00 2   61.9789400    -414570.000
   1023.000   1243.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12400.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.485897470D+04-6.235394464D+01
Na2O(a)            Alpha. Gurvich,1982 pt1 p320 pt2 p360.
 1 tpis82 NA  2.00O   1.00    0.00     0.00     0.00 3   61.9789400    -414570.000
   1243.000   1405.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12400.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.377652960D+04-6.148311196D+01
Na2O(L)            Liquid. Gurvich,1982 pt1 p320 pt2 p360.
 1 tpis82 NA  2.00O   1.00    0.00     0.00     0.00 4   61.9789400    -414570.000
   1405.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12400.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.944674950D+04-5.840141793D+01
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Na2O2(b)          Beta. Gurvich,1982 pt1 p323 pt2 p363.
 2 tpis82 NA  2.00O   2.00     0.00     0.00     0.00 1   77.9783400    -512000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15694.000
-8.122024280D+05 1.451270156D+04-1.058114918D+02 4.802903390D-01-1.057140356D-03
 1.219343411D-06-5.728124010D-10                 -1.295899700D+05 5.525239130D+02
    500.000    785.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15694.000
-1.051839392D+05 0.000000000D+00 1.054275850D+01 4.638430480D-03 4.381769570D-09
 0.000000000D+00 0.000000000D+00                 -6.528135100D+04-5.064487560D+01
Na2O2(a)          Alpha. Gurvich,1982 pt1 p323 pt2 p363.
 1 tpis82 NA  2.00O   2.00     0.00     0.00     0.00 2   77.9783400    -512000.000
    785.000    948.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15694.000
 0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.546547070D+04-6.641239933D+01
Na2O2(L)          Liquid. Gurvich,1982 pt1 p323 pt2 p363.
 1 tpis82 NA  2.00O   2.00     0.00     0.00     0.00 3   77.9783400    -512000.000
    948.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15694.000
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.581522070D+04-8.156770675D+01
Na2S(cr)          Below lambda trans. Chase,1998 pp1667-9.
 2 j 3/78 NA  2.00S   1.00     0.00     0.00     0.00 1   78.0445400    -366100.000
    298.150    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
-4.541358110D+05 4.959201300D+03-1.171687783D+01 4.586680300D-02-4.501505030D-05
 1.801159260D-08 0.000000000D+00                 -7.199330320D+04 8.057734670D+01
    700.000   1276.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
-3.527498880D+09 2.408466098D+07-6.783369110D+04 1.008062531D+02-8.320894540D-02
 3.611294520D-05-6.422558180D-09                 -1.325119033D+08 4.212898800D+05
Na2S(cr)          Above lambda trans. Chase,1998 pp1667-9.
 1 j 3/78 NA  2.00S   1.00     0.00     0.00     0.00 2   78.0445400    -366100.000
   1276.000   1445.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 8.868348820D+08 0.000000000D+00-2.045962174D+03 1.675387705D+00-3.752802310D-04
 0.000000000D+00 0.000000000D+00                  2.169500522D+06 1.309983113D+04
Na2S(L)           Chase,1998 pp1667-9.
 1 j 3/78 NA  2.00S   1.00     0.00     0.00     0.00 3   78.0445400    -366100.000
   1445.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 1.107076665D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.262953690D+04-4.848427350D+01
Na2SO3(cr)        Crystal. Barin,1989 pt2 p1002.
 1 bar 89 NA  2.00S   1.00O   3.00     0.00     0.00 1  126.0427400   -1100802.000
    298.150   1184.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 1.290193602D+01 5.233511440D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.364746191D+05-5.751819280D+01
Na2SO3(L)         Liquid. Barin,1989 pt2 p1002.
 1 bar 89 NA  2.00S   1.00O   3.00     0.00     0.00 2  126.0427400   -1100802.000
   1184.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 2.188992496D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.403382187D+05-1.123000267D+02
Na2SO4(V)         Rhombic. Gurvich,1982 pt1 p346 pt2 p384.
 1 tpis82 NA  2.00S   1.00O   4.00     0.00     0.00 1  142.0421400   -1387900.000
    200.000    458.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23204.000
-8.689043820D+05 1.449012038D+04-9.087576950D+01 3.621919930D-01-5.592870850D-04
 3.463421130D-07 0.000000000D+00                 -2.371450313D+05 4.932876470D+02
Na2SO4(IV)        Rhombic. Gurvich,1982 pt1 p346 pt2 p384.
 1 tpis82 NA  2.00S   1.00O   4.00     0.00     0.00 2  142.0421400   -1387900.000
    458.000    514.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23204.000
-1.455046659D+05 0.000000000D+00 1.308904554D+01 1.323950539D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.718682018D+05-6.127355231D+01
Na2SO4(I)         Hexagonal. Gurvich,1982 pt1 p346 pt2 p384.
 1 tpis82 NA  2.00S   1.00O   4.00     0.00     0.00 3  142.0421400   -1387900.000
    514.000   1157.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23204.000
 0.000000000D+00 0.000000000D+00 2.503069934D+01-1.581223668D-02 1.591831629D-05
 0.000000000D+00 0.000000000D+00                 -1.732950425D+05-1.201603231D+02
Na2SO4(L)         Liquid. Gurvich,1982 pt1 p346 pt2 p384.
 1 tpis82 NA  2.00S   1.00O   4.00     0.00     0.00 4  142.0421400   -1387900.000
   1157.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          23204.000
 0.000000000D+00 0.000000000D+00 2.453542061D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.722609524D+05-1.218642150D+02
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Na3ALF6(a)          Monoclinic. Gurvich,1982 pt1 p361 pt2 p394.
 2 tpis82 NA  3.00AL  1.00F   6.00    0.00    0.00 1  209.9412672   -3322400.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         38070.000
 1.564580425D+07-2.923454204D+05 2.211217567D+03-8.502636700D+00 1.825363780D-02
-2.047448239D-05 9.409455420D-09                 9.119433290D+05-1.157646461D+04
    500.000    838.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         38070.000
-1.416702978D+05 0.000000000D+00 2.315158739D+01 1.479360403D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.076260850D+05-1.084672805D+02
Na3ALF6(b)          Cubic. Gurvich,1982 pt1 p361 pt2 p394.
 1 tpis82 NA  3.00AL  1.00F   6.00    0.00    0.00 2  209.9412672   -3322400.000
    838.000   1286.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         38070.000
 0.000000000D+00 0.000000000D+00 2.624279723D+01 7.980987454D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.065549160D+05-1.221511986D+02
Na3ALF6(L)          Liquid. Gurvich,1982 pt1 p361 pt2 p394.
 1 tpis82 NA  3.00AL  1.00F   6.00    0.00    0.00 3  209.9412672   -3322400.000
   1286.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         38070.000
 0.000000000D+00 0.000000000D+00 4.702622283D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.129238590D+05-2.499831311D+02
Na5AL3F14(cr)       Tetragonal. Gurvich,1982 pt1 p362 pt2 p395.
 2 tpis82 NA  5.00AL  3.00F  14.00    0.00    0.00 1  461.8711088   -7555000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         80830.000
-2.302157125D+07 4.240174110D+05-3.188373880D+03 1.288416515D+01-2.796179544D-02
 3.169729270D-05-1.469118702D-08                -2.832459181D+06 1.667109223D+04
    500.000   1010.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         80830.000
-8.720901540D+05 0.000000000D+00 6.109021050D+01 1.113784152D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.302863450D+05-2.943295261D+02
Na5AL3F14(L)        Liquid. Gurvich,1982 pt1 p362 pt2 p395.
 1 tpis82 NA  5.00AL  3.00F  14.00    0.00    0.00 2  461.8711088   -7555000.000
   1010.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         80830.000
 0.000000000D+00 0.000000000D+00 1.171446062D+02 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.528147600D+05-6.431511436D+02
Nb(cr)              Crystal. Ref-Elm. Chase,1998 pp1675-8.
 3 j12/73 NB  1.00    0.00    0.00    0.00    0.00 1   92.9063800          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5241.000
-4.254811710D+04 3.875297090D+02 1.184449739D+00 4.507436620D-03-5.232091980D-06
 3.513452460D-09-9.507605800D-13                -2.864449323D+03-2.442975114D+00
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5241.000
 2.527695630D+07-1.085720528D+05 1.929168202D+02-1.727427651D-01 8.671274570D-05
-2.266162374D-08 2.437387316D-12                 6.472317770D+05-1.284027328D+03
   2000.000   2750.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5241.000
 9.016788690D+08-1.888649522D+06 1.578845370D+03-6.588882220D-01 1.416307803D-04
-1.396561356D-08 4.411624050D-13                 1.264760547D+07-1.175157316D+04
Nb(L)               Liquid. Ref-Elm. Chase,1998 pp1675-8.
 1 j12/73 NB  1.00    0.00    0.00    0.00    0.00 2   92.9063800          0.000
   2750.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5241.000
 0.000000000D+00 0.000000000D+00 4.025733326D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.427029683D+03-1.857965621D+01
NbO(cr)             Cubic. Gurvich,1982 pt1 p75 pt2 p77.
 1 tpis82 NB  1.00O   1.00    0.00    0.00    0.00 1  108.9057800     -406000.000
    298.150   2217.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7200.000
-4.430808310D+04 0.000000000D+00 5.073540112D+00 1.194297680D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.054466650D+04-2.397978879D+01
NbO(L)              Liquid. Gurvich,1982 pt1 p75 pt2 p77.
 1 tpis82 NB  1.00O   1.00    0.00    0.00    0.00 2  108.9057800     -406000.000
   2217.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7200.000
 0.000000000D+00 0.000000000D+00 7.817658527D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.765976820D+04-3.975547844D+01
NbOCL3(cr)          Barin,1989 pt2 p1030. Wagman,1982 p207.
 1 bar 89 NB  1.00O   1.00CL  3.00    0.00    0.00 1  215.2647800     -879500.000
    298.150    702.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
-1.822304138D+05 4.828593360D+02 1.341861113D+01 7.546458250D-03-1.198129404D-05
 9.997155720D-09-3.425554610D-12                -1.133897355D+05-6.057973360D+01
NbO2(II)            Tetragonal. Gurvich,1982 pt1 p78 pt2 p80.
 2 tpis82 NB  1.00O   2.00    0.00    0.00    0.00 1  124.9051800     -795000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9267.000
-3.914505940D+06 7.500739880D+04-5.854724840D+02 2.416380822D+00-5.358130280D-03
 6.172498470D-06-2.893870224D-09                -4.324424750D+05 3.040766836D+03
    500.000   1082.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9267.000
-2.074227934D+05 0.000000000D+00 1.075172627D+01-7.363421090D-03 7.988904160D-06
 0.000000000D+00 0.000000000D+00                -9.926049480D+04-5.405566340D+01
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NbO2(I)             Tetragonal. Gurvich,1982 pt1 p78 pt2 p80.
 1 tpis82 NB  1.00O   2.00     0.00     0.00     0.00 2  124.9051800     -795000.000
   1082.000   2360.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9267.000
-2.470500366D+05 0.000000000D+00 1.027937906D+01 1.610437657D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.951665200D+04-5.395968051D+01
NbO2(L)             Liquid. Gurvich,1982 pt1 p78 pt2 p80.
 1 tpis82 NB  1.00O   2.00     0.00     0.00     0.00 3  124.9051800     -795000.000
   2360.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            9267.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.406789930D+04-6.330929540D+01
Nb2O5(cr)           Monoclinic. Gurvich,1982 pt1 p81 pt2 p82.
 2 tpis82 NB  2.00O   5.00     0.00     0.00     0.00 1  265.8097600    -1897000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           22240.000
 2.640209200D+07-4.944721050D+05 3.755171780D+03-1.472158158D+01 3.190561080D-02
-3.609939830D-05 1.669960716D-08                 1.993996743D+06-1.963185769D+04
    500.000   1783.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           22240.000
 2.666894830D+05 0.000000000D+00-3.157808421D+00 7.820838380D-02-9.622327490D-05
 5.100828450D-08-9.357603760D-12                 -2.290426814D+05 1.650612260D+01
Nb2O5(L)            Liquid. Gurvich,1982 pt1 p81 pt2 p82.
 1 tpis82 NB  2.00O   5.00     0.00     0.00     0.00 2  265.8097600    -1897000.000
   1783.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           22240.000
 0.000000000D+00 0.000000000D+00 2.405433393D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.279011100D+05-1.212064449D+02
Ni(cr)              Crystal Ref-Elm. <lambda trans 631K. Chase,1998 pp1697-700.
 2 j12/76 NI  1.00    0.00     0.00     0.00     0.00 1   58.6934000           0.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           4786.000
-7.689131090D+05 1.433956218D+04-1.042751331D+02 3.926261320D-01-6.986906890D-04
 4.906078910D-07 0.000000000D+00                 -6.543789970D+04 5.511391170D+02
    400.000    631.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           4786.000
-3.345887340D+08 3.424527970D+06-1.394425564D+04 2.825654843D+01-2.847789131D-02
 1.142789828D-05 0.000000000D+00                 -1.750250768D+07 8.179861400D+04
Ni(cr)              Crystal Ref-Elm. >lambda trans 631K. Chase,1998 pp1697-700.
 2 j12/76 NI  1.00    0.00     0.00     0.00     0.00 2   58.6934000           0.000
    631.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           4786.000
 1.036354737D+09-6.813278550D+06 1.854367615D+04-2.673006535D+01 2.153531609D-02
-9.192464140D-06 1.624332987D-09                 3.771960950D+07-1.157617522D+05
   1200.000   1728.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           4786.000
 2.518440662D+09-9.895465230D+06 1.609737530D+04-1.386478566D+01 6.671320910D-03
-1.698988160D-06 1.788537986D-10                 5.987658740D+07-1.087743318D+05
Ni(L)               Liquid. Ref-Elm. Chase,1998 pp1697-700.
 1 j12/76 NI  1.00    0.00     0.00     0.00     0.00 3   58.6934000           0.000
   1728.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           4786.000
 0.000000000D+00 0.000000000D+00 4.679890938D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.216258550D+02-2.335474714D+01
NiS(b)              Beta. Chase,1998 pp1704-6.
 1 j12/76 NI  1.00S   1.00     0.00     0.00     0.00 1   90.7584000      -87864.000
    200.000    652.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8465.000
 9.281477840D+04-2.341897035D+03 2.156233266D+01-5.304222560D-02 9.993984760D-05
-9.111093130D-08 3.288570290D-11                 -1.702746009D+03-1.117002463D+02
NiS(a)              ALpha. Chase,1998 pp1704-6.
 1 j12/76 NI  1.00S   1.00     0.00     0.00     0.00 2   90.7584000      -87864.000
    652.000   1249.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8465.000
 2.424566967D+05-1.320914239D+03 7.077218200D+00 9.029383650D-05 2.068184040D-06
-6.559770780D-10 8.194048850D-14                 -3.434758890D+03-3.562024750D+01
NiS(L)              Liquid. Chase,1998 pp1704-6.
 1 j12/76 NI  1.00S   1.00     0.00     0.00     0.00 3   90.7584000      -87864.000
   1249.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8465.000
 0.000000000D+00 0.000000000D+00 9.233977709D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.105334670D+04-4.576765033D+01
NiS2(cr)            Crystal. Chase,1998 pp1708-10.
 1 j 3/77 NI  1.00S   2.00     0.00     0.00     0.00 1  122.8234000     -131377.600
    298.150   1280.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
-1.676910840D+03 1.842877438D+01 7.671341480D+00 2.663682250D-03-1.892467189D-07
 1.078337009D-10-2.438956464D-14                 -1.831575942D+04-3.578715100D+01
NiS2(L)             Liquid. Chase,1998 pp1708-10.
 1 j 3/77 NI  1.00S   2.00     0.00     0.00     0.00 2  122.8234000     -131377.600
   1280.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 1.094496248D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.234477669D+04-4.971946503D+01
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Appendix D (*continued*)

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Ni3S2(a)          Alpha. Pankratz,1987 p225-6. Chase,1998 pp1711-3 12/83.
 1 g12/00 NI  3.00S   2.00     0.00     0.00     0.00 1  240.2102000    -217986.400
    200.000    834.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21155.978
-6.710970630D+05 9.870810610D+03-5.338151110D+01 2.311567743D-01-3.933292800D-04
 3.340311640D-07-1.054748249D-10                -7.620212300D+04 2.954015489D+02
Ni3S2(b)          Beta. Pankratz,1987 p225-6.
 1 g12/00 NI  3.00S   2.00     0.00     0.00     0.00 2  240.2102000    -217986.400
    834.000   1064.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21155.978
-5.072819670D+04 0.000000000D+00 2.665250520D+01-4.426613790D-03 3.885431570D-07
 0.000000000D+00 0.000000000D+00                -3.142142347D+04-1.348956828D+02
Ni3S2(L)          Liquid. Pankratz,1987 p225-6.
 1 g12/00 NI  3.00S   2.00     0.00     0.00     0.00 3  240.2102000    -217986.400
   1064.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21155.978
 0.000000000D+00 0.000000000D+00 2.274539329D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.720113051D+04-1.099086536D+02
Ni3S4(cr)         Crystal. Chase,1998 p1714.
 1 j 3/77 NI  3.00S   4.00     0.00     0.00     0.00 1  304.3402000    -301115.000
    298.150   1100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 7.214883180D+03-7.806476430D+01 1.500658024D+01 1.653827825D-02 8.768311110D-07
-5.301784170D-10 1.279272852D-13                -4.096266670D+04-6.825975310D+01
P(cr)             White. Ref-Elm. Gurvich,1989 pt1 p395 pt2 p326. Chase,1998a.
 1 tpis89 P   1.00    0.00     0.00     0.00     0.00 1   30.9737610         0.000
    195.400    317.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5360.000
-4.761561170D+06 1.135422659D+05-1.120481079D+03 5.889005080D+00-1.727002916D-02
 2.689248597D-05-1.737186959D-08                -4.829321490D+05 5.551556600D+03
P(L)              Liquid. Ref-Elm. Gurvich,1989 pt1 p395 pt2 p326.
 1 tpis89 P   1.00    0.00     0.00     0.00     0.00 2   30.9737610         0.000
    317.300   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5360.000
 0.000000000D+00 0.000000000D+00 3.141496011D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.621436240D+02-1.272272999D+01
P4O10(cr)         Crystal. Gurvich,1989 pt1 p417 pt2 p270.
 2 tpis89 P   4.00O  10.00     0.00     0.00     0.00 1  283.8890440   -3010100.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         34220.000
-2.910475984D+04 0.000000000D+00 5.209612140D+00 7.058407940D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.668178470D+05-2.310786251D+01
    298.150    699.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         34220.000
 0.000000000D+00 0.000000000D+00 5.461897334D+00 8.078166964D-02-4.072398734D-05
 0.000000000D+00 0.000000000D+00                -3.668889200D+05-2.561194012D+01
P4O10(L)          Liquid. Gurvich,1989 pt1 p417 pt2 p270.
 1 tpis89 P   4.00O  10.00     0.00     0.00     0.00 3  283.8890440   -3010100.000
    699.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         34220.000
 0.000000000D+00 0.000000000D+00 4.450051777D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.765523910D+05-2.311704609D+02
Pb(cr)            Cubic. Ref-Elm. Gurvich,1991 pt1 p400 pt2 p337.
 1 tpis91 PB  1.00    0.00     0.00     0.00     0.00 1  207.2000000         0.000
    200.000    600.6507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6870.000
-6.149670140D+05 1.065718060D+04-7.129898940D+01 2.668406702D-01-5.182017320D-04
 5.238665090D-07-2.151645616D-10                -4.974077560D+04 3.855826030D+02
Pb(L)             Liquid. Ref-Elm. Gurvich,1991 pt1 p400 pt2 p337.
 1 tpis91 PB  1.00    0.00     0.00     0.00     0.00 2  207.2000000         0.000
    600.650   3600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6870.000
-3.798179327D+04 0.000000000D+00 4.364298076D+00-1.236392764D-03 4.946773773D-07
-5.231817630D-11 0.000000000D+00                -8.887330420D+02-1.619559677D+01
PbBr2(cr)         Rhombic Crystal. Gurvich,1991 pt1 p435 pt2 p361.
 2 tpis91 PB  1.00BR  2.00     0.00     0.00     0.00 1  367.0080000    -276700.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19230.000
 0.000000000D+00 0.000000000D+00 6.565717260D+00 1.959605208D-02-3.191530530D-05
 0.000000000D+00 0.000000000D+00                -3.582576310D+04-2.245707569D+01
    298.150    644.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19230.000
 8.046174699D+04 0.000000000D+00 6.899264058D+00 5.925905435D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.532970360D+04-2.124769272D+01
PbBr2(L)          Liquid. Gurvich,1991 pt1 p435 pt2 p361.
 1 tpis91 PB  1.00BR  2.00     0.00     0.00     0.00 2  367.0080000    -276700.000
    644.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19230.000
 0.000000000D+00 0.000000000D+00 1.347042700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.648036370D+04-5.695842618D+01
PbCL2(cr)         Rhombic Crystal. Gurvich,1991 pt1 p428 pt2 p356.
 1 tpis91 PB  1.00CL  2.00     0.00     0.00     0.00 1  278.1060000    -359400.000
    200.000    774.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17150.000
 2.697281121D+06-4.212942350D+04 2.651641932D+02-7.891350070D-01 1.316948609D-03
-1.123561948D-06 3.854416550D-10                1.522766773D+05-1.434661776D+03
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PbCL2(L)            Liquid. Gurvich,1991 pt1 p428 pt2 p356.
 1 tpis91 PB  1.00CL  2.00     0.00     0.00     0.00 2  278.1060000     -359400.000
    774.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17150.000
 0.000000000D+00 0.000000000D+00 1.335015533D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.613690180D+04-5.953419614D+01
PbF2(II)            Rhombic Crystal(II). Gurvich,1991 pt1 p421 pt2 p351.
 1 tpis91 PB  1.00F   2.00     0.00     0.00     0.00 1  245.1968064     -676000.000
    298.150     583.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15000.000
 1.363880734D+04 0.000000000D+00 7.104086711D+00 4.806777549D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.358963280D+04-2.908385048D+01
PbF2(I)             Cubic Crystal(I). Gurvich,1991 pt1 p421 pt2 p351.
 2 tpis91 PB  1.00F   2.00     0.00     0.00     0.00 2  245.1968064     -676000.000
    583.000     716.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15000.000
-7.862766417D+07 0.000000000D+00 1.154013526D+03-2.413080386D+00 1.453441514D-03
 0.000000000D+00 0.000000000D+00                -5.720487300D+05-6.285579567D+03
    716.000    1103.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15000.000
 3.516663038D+07 0.000000000D+00-1.580925394D+02 1.905776769D-01-5.650555475D-05
 0.000000000D+00 0.000000000D+00                 4.370723820D+04 9.735936305D+02
PbF2(L)             Liquid. Gurvich,1991 pt1 p421 pt2 p351.
 1 tpis91 PB  1.00F   2.00     0.00     0.00     0.00 3  245.1968064     -676000.000
   1103.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15000.000
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.458950020D+04-6.282775717D+01
PbI2(cr)            Hexagonal Crystal. Gurvich,1991 pt1 p441 pt2 p366.
 2 tpis91 PB  1.00I   2.00     0.00     0.00     0.00 1  461.0089400     -176000.000
    100.000     298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19500.000
-6.615857400D+03 0.000000000D+00 8.879658690D+00 1.758307313D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.391562477D+04-3.012466437D+01
    298.150     683.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19500.000
 4.428402876D+04 0.000000000D+00 7.731062925D+00 3.690055096D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.348831172D+04-2.387008226D+01
PbI2(L)             Liquid. Gurvich,1991 pt1 p441 pt2 p366.
 1 tpis91 PB  1.00I   2.00     0.00     0.00     0.00 2  461.0089400     -176000.000
    683.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19500.000
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.355165613D+04-5.237973135D+01
PbO(II-r)           Tetragonal (II-red).Gurvich,1991 pt1 p409 pt2 p343.
 2 tpis91 PB  1.00O   1.00     0.00     0.00     0.00 1  223.1994000     -218600.000
    100.000     298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9225.000
 0.000000000D+00 0.000000000D+00 8.050624580D-01 2.884978163D-02-4.302158100D-05
 0.000000000D+00 0.000000000D+00                -2.743361905D+04-3.117085753D+00
    298.150     762.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9225.000
-6.651023332D+03 0.000000000D+00 4.939557472D+00 2.406636110D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.789339075D+04-2.073932502D+01
PbO(I-y)            Rhombic (I-yellow).Gurvich,1991 pt1 p409 pt2 p343.
 1 tpis91 PB  1.00O   1.00     0.00     0.00     0.00 2  223.1994000     -218600.000
    762.000    1160.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9225.000
-3.360390450D+04 0.000000000D+00 5.407414267D+00 1.595644241D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.802576574D+04-2.321766400D+01
PbO(L)              Liquid.Gurvich,1991 pt1 p409 pt2 p343.
 1 tpis91 PB  1.00O   1.00     0.00     0.00     0.00 3  223.1994000     -218600.000
   1160.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9225.000
 0.000000000D+00 0.000000000D+00 7.817658527D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.664258145D+04-3.570913839D+01
PbO2(cr)            Tetragonal. Gurvich,1991 pt1 p415 p52 p346.
 2 tpis91 PB  1.00O   2.00     0.00     0.00     0.00 1  239.1988000     -276000.000
    100.000     298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10962.000
 0.000000000D+00 0.000000000D+00 1.007530476D-01 4.035527600D-02-5.395750800D-05
 0.000000000D+00 0.000000000D+00                -3.454199070D+04-1.557803514D+00
    298.150    1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10962.000
-2.593057198D+05 0.000000000D+00 1.010402297D+01 5.003301457D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.709944890D+04-5.052640331D+01
PbS(cr)             Cubic. Gurvich,1991 pt1 p445 p52 p370.
 2 tpis91 PB  1.00S   1.00     0.00     0.00     0.00 1  239.2650000      -99474.800
    100.000     298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11510.000
-1.110196130D+04 0.000000000D+00 5.788552660D+00 9.715425300D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.377027529D+04-2.236417313D+01
    298.150    1386.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11510.000
-7.529006520D+04 0.000000000D+00 7.331760982D+00-2.262310106D-03 1.609234940D-06
 0.000000000D+00 0.000000000D+00                -1.431615352D+04-3.062514348D+01
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PbS(L)              Liquid. Gurvich,1991 pt1 p445 p52 p370.
 1 tpis91 PB  1.00S   1.00     0.00     0.00     0.00 2  239.2650000     -99474.800
   1386.500   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          11510.000
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.007241100D+04-3.316574241D+01
Pb2O3(cr)           Monoclinic. Gurvich,1991 pt1 p417 pt2 p348.
 2 tpis91 PB  2.00O   3.00     0.00     0.00     0.00 1  462.3982000     -491700.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20880.000
 0.000000000D+00 0.000000000D+00 1.574967406D+00 6.633690300D-02-9.449445980D-05
 0.000000000D+00 0.000000000D+00                -6.172080000D+04-6.282642160D+00
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20880.000
-3.314687215D+05 0.000000000D+00 1.505921576D+01 5.443495768D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.498118220D+04-7.101946635D+01
Pb3O4(cr)           Tetragonal. Gurvich,1991 pt1 p418 pt2 p349.
 1 tpis91 PB  3.00O   4.00     0.00     0.00     0.00 1  685.5976000     -720000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          29830.000
 7.031601470D+06-8.770415980D+04 4.195886490D+02-9.058738460D-01 1.138287119D-03
-7.358926050D-07 1.922732625D-10                3.431611340D+05-2.394229365D+03
Rb(cr)              Cubic. Ref-Elm. Cox,1989 p260. Chase,1998a p1849 12/83.
 1 coda89 RB  1.00    0.00     0.00     0.00     0.00 1   85.4678000         0.000
    100.000    312.4707 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7489.000
-1.693678854D+05 5.116764690D+03-5.686760910D+01 3.403543550D-01-9.347996350D-04
 1.017512352D-06 0.000000000D+00                -2.164547399D+04 2.805351095D+02
Rb(L)               Liquid. Ref-Elm. Cox,1989 p260.
 2 coda89 RB  1.00    0.00     0.00     0.00     0.00 2   85.4678000         0.000
    312.470   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7489.000
 2.365752770D+04 2.865695009D+02 1.546589030D+00 5.164698120D-03-6.065846790D-06
 3.347806150D-09-5.178101420D-13                -1.933656171D+03 1.060307276D+00
   1000.000   2100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           7489.000
-3.672685780D+05 1.779065421D+03-3.414096790D-01 5.322070690D-03-4.262302730D-06
 1.699676170D-09-4.416789770D-14                -1.110894373D+04 1.477099469D+01
RbBO2(b)            Gurvich,1982 pt1 p458 pt2 p482.
 2 tpis82 RB  1.00B   1.00O   2.00     0.00     0.00 1  128.2776000     -975000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13310.000
 1.320700184D+06-2.114255330D+04 1.338015047D+02-3.804509820D-01 6.570568430D-04
-5.884791840D-07 2.152384344D-10                -2.010026759D+04-7.254857290D+02
    500.000    968.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13310.000
-1.553422560D+05 0.000000000D+00 9.425074910D+00 3.853433670D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.207672511D+05-4.437890740D+01
RbBO2(a)            Gurvich,1982 pt1 p458 pt2 p482.
 1 tpis82 RB  1.00B   1.00O   2.00     0.00     0.00 2  128.2776000     -975000.000
    968.000   1133.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13310.000
 0.000000000D+00 0.000000000D+00 1.298934032D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.222516025D+05-6.507104425D+01
RbBO2(L)            Gurvich,1982 pt1 p458 pt2 p482.
 1 tpis82 RB  1.00B   1.00O   2.00     0.00     0.00 3  128.2776000     -975000.000
   1133.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13310.000
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.235650894D+05-9.307583456D+01
RbBr(cr)            Cubic. Gurvich,1982 pt1 p445 pt2 p469.
 1 tpis82 RB  1.00BR  1.00     0.00     0.00     0.00 1  165.3718000     -394770.000
    200.000    965.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13060.000
-5.724525880D+04 9.082670760D+02 4.275929780D-01 1.751269798D-02-2.421969308D-05
 1.854230436D-08-5.603980870D-12                -5.357247720D+04 9.232346100D+00
RbBr(L)             Liquid. Gurvich,1982 pt1 p445 pt2 p469.
 1 tpis82 RB  1.00BR  1.00     0.00     0.00     0.00 2  165.3718000     -394770.000
    965.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13060.000
 0.000000000D+00 0.000000000D+00 8.755777550D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.852456540D+04-3.604442573D+01
RbCL(cr)            Cubic. Gurvich,1982 pt1 p441 pt2 p466.
 1 tpis82 RB  1.00CL  1.00     0.00     0.00     0.00 1  120.9208000     -435220.000
    200.000    997.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12160.000
-5.731907690D+04 4.298433250D+02 4.955874940D+00 9.930643910D-04 3.857679940D-06
-4.516778380D-09 1.683809372D-12                -5.653364290D+04-1.609477359D+01
RbCL(L)             Liquid. Gurvich,1982 pt1 p441 pt2 p466.
 1 tpis82 RB  1.00CL  1.00     0.00     0.00     0.00 2  120.9208000     -435220.000
    997.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          12160.000
 0.000000000D+00 0.000000000D+00 8.827940552D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.345006300D+04-3.845805693D+01
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RbF(cr)            Cubic. Gurvich,1982 pt1 p438 pt2 p463.
 1 tpis82 RB  1.00F   1.00    0.00    0.00    0.00 1  104.4662032    -559700.000
    298.150   1068.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10900.000
 5.640741306D+03 0.000000000D+00 5.092663308D+00 3.129949931D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.895462790D+04-2.057230003D+01
RbF(L)             Liquid. Gurvich,1982 pt1 p438 pt2 p463.
 1 tpis82 RB  1.00F   1.00    0.00    0.00    0.00 2  104.4662032    -559700.000
   1068.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10900.000
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.775044270D+04-3.835948403D+01
RbH(cr)            Cubic. Gurvich,1982 pt1 p434 pt2 p458.
 1 tpis82 RB  1.00H   1.00    0.00    0.00    0.00 1   86.4757400     -52300.000
    298.150    858.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9100.000
-6.384020225D+04 0.000000000D+00 4.263149602D+00 3.963552873D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.951554350D+03-1.816921793D+01
RbH(L)             Liquid. Gurvich,1982 pt1 p434 pt2 p458.
 1 tpis82 RB  1.00H   1.00    0.00    0.00    0.00 2   86.4757400     -52300.000
    858.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9100.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.893290150D+03-2.833905350D+01
RbI(cr)            Cubic. Gurvich,1982 pt1 p448 pt2 p472.
 1 tpis82 RB  1.00I   1.00    0.00    0.00    0.00 1  212.3722700    -333600.000
    200.000    929.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13340.000
-1.871461077D+05 2.207646572D+03-3.199388250D+00 1.739850250D-02-1.184152545D-05
 3.313152520D-09 3.472456000D-13                -5.305010310D+04 3.417793530D+01
RbI(L)             Liquid. Gurvich,1982 pt1 p448 pt2 p472.
 1 tpis82 RB  1.00I   1.00    0.00    0.00    0.00 2  212.3722700    -333600.000
    929.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13340.000
 0.000000000D+00 0.000000000D+00 8.671587382D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.112940250D+04-3.435941214D+01
RbNO2(I)           Cubic. Gurvich,1982 pt1 p453 pt2 p477.
 1 tpis82 RB  1.00N   1.00O   2.00    0.00    0.00 1  131.4733000    -367000.000
    298.150    695.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23400.000
 0.000000000D+00 0.000000000D+00 9.108895172D+00 3.333690139D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.700369140D+04-3.340874045D+01
RbNO2(L)           Liquid. Gurvich,1982 pt1 p453 pt2 p477.
 1 tpis82 RB  1.00N   1.00O   2.00    0.00    0.00 2  131.4733000    -367000.000
    695.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23400.000
 0.000000000D+00 0.000000000D+00 1.250825364D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.710583050D+04-5.124298955D+01
RbNO3(IV)          Hexagonal. Gurvich,1982 pt1 p455 pt2 p479.
 1 tpis82 RB  1.00N   1.00O   3.00    0.00    0.00 1  147.4727000    -494700.000
    200.000    437.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19640.000
 1.211253372D+07-2.028159094D+05 1.325899840D+03-4.151421820D+00 6.401606600D-03
-3.822822630D-06 0.000000000D+00                8.768873850D+05-7.162144700D+03
RbNO3(III)         Cubic. Gurvich,1982 pt1 p455 pt2 p479.
 1 tpis82 RB  1.00N   1.00O   3.00    0.00    0.00 2  147.4727000    -494700.000
    437.000    493.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19640.000
 0.000000000D+00 0.000000000D+00 9.120561524D+00 1.643716828D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.277664760D+04-3.918776498D+01
RbNO3(II)          Hexagonal. Gurvich,1982 pt1 p455 pt2 p479.
 1 tpis82 RB  1.00N   1.00O   3.00    0.00    0.00 3  147.4727000    -494700.000
    493.000    556.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19640.000
 0.000000000D+00 0.000000000D+00 1.078616780D+02-2.821762196D-01 0.000000000D+00
 3.922207081D-07 0.000000000D+00                -8.057470150D+04-5.191016028D+02
RbNO3(I)           Cubic. Gurvich,1982 pt1 p455 pt2 p479.
 1 tpis82 RB  1.00N   1.00O   3.00    0.00    0.00 4  147.4727000    -494700.000
    556.000    583.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19640.000
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.449488250D+04-8.253206472D+01
RbNO3(L)           Liquid. Gurvich,1982 pt1 p455 pt2 p479.
 1 tpis82 RB  1.00N   1.00O   3.00    0.00    0.00 5  147.4727000    -494700.000
    583.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19640.000
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.394163280D+04-8.158309442D+01
RbOH(b)            Beta.  Gurvich,1997.
 1 g 8/97 RB  1.00O   1.00H   1.00    0.00    0.00 1  102.4751400    -418800.000
    298.150    508.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13500.000
 0.000000000D+00 0.000000000D+00 6.589925323D+00 5.731305874D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.258929920D+04-2.794998878D+01
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RbOH(c)            Gamma. Gurvich,1997.
 1 g 8/97 RB  1.00O   1.00H   1.00     0.00     0.00 2  102.4751400     -418800.000
    508.000    658.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13500.000
 0.000000000D+00 0.000000000D+00 9.140646893D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.248404970D+04-3.962855491D+01
RbOH(L)            Liquid. Gurvich,1997.
 1 g 8/97 RB  1.00O   1.00H   1.00     0.00     0.00 3  102.4751400     -418800.000
    658.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13500.000
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.231326390D+04-4.597096049D+01
RbO2(b)            Beta,hexagonal. Gurvich,1982 pt1 p430 pt2 p453.
 1 tpis82 RB  1.00O   2.00    0.00     0.00     0.00 1  117.4666000     -279100.000
    200.000    423.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16760.000
-5.914373690D+05 9.356154690D+03-5.173703230D+01 1.872603527D-01-2.664203296D-04
 1.581120816D-07 0.000000000D+00                 -7.971547560D+04 2.930911089D+02
RbO2(a)            Alpha,cubic. Gurvich,1982 pt1 p430 pt2 p453.
 1 tpis82 RB  1.00O   2.00    0.00     0.00     0.00 2  117.4666000     -279100.000
    423.000    813.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16760.000
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.680173520D+04-4.488768335D+01
RbO2(L)            Liquid. Gurvich,1982 pt1 p430 pt2 p453.
 1 tpis82 RB  1.00O   2.00    0.00     0.00     0.00 3  117.4666000     -279100.000
    813.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          16760.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.544940050D+04-5.145193248D+01
Rb2CO3(a)          Alpha,monoclinic. Gurvich,1982 pt1 p457 pt2 p481.
 1 tpis82 RB  2.00C   1.00O   3.00     0.00     0.00 1  230.9445000    -1132600.000
    200.000    576.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24480.000
-1.377487286D+06 2.415872404D+04-1.620555595D+02 6.425655960D-01-1.249826185D-03
 1.304525231D-06-5.552423710D-10                 -2.500033904D+05 8.719586300D+02
Rb2CO3(b)          Beta,hexagonal. Gurvich,1982 pt1 p457 pt2 p481.
 1 tpis82 RB  2.00C   1.00O   3.00     0.00     0.00 2  230.9445000    -1132600.000
    576.000   1146.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24480.000
 0.000000000D+00 0.000000000D+00 1.355678206D+01 8.280944999D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.405896222D+05-5.801044809D+01
Rb2CO3(L)          Liquid. Gurvich,1982 pt1 457 pt2 p481.
 1 tpis82 RB  2.00C   1.00O   3.00     0.00     0.00 3  230.9445000    -1132600.000
   1146.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24480.000
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.442630744D+05-1.235531008D+02
Rb2O(c)            Gamma,cubic. Gurvich,1982 pt1 p431 pt2 p454.
 1 tpis82 RB  2.00O   1.00    0.00     0.00     0.00 1  186.9350000     -338000.000
    298.150    543.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15600.000
 0.000000000D+00 0.000000000D+00 6.190743652D+00 9.087246272D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.290149280D+04-2.294776447D+01
Rb2O(b)            Beta,cubic. Gurvich,1982 pt1 p431 pt2 p454.
 1 tpis82 RB  2.00O   1.00    0.00     0.00     0.00 2  186.9350000     -338000.000
    543.000    613.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15600.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.464679770D+04-5.461093903D+01
Rb2O(a)            Alpha,hexagonal. Gurvich,1982 pt1 p431 pt2 p454.
 1 tpis82 RB  2.00O   1.00    0.00     0.00     0.00 3  186.9350000     -338000.000
    613.000    778.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15600.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.416571100D+04-5.382613205D+01
Rb2O(L)            Liquid. Gurvich,1982 pt1 p431 pt2 p454.
 1 tpis82 RB  2.00O   1.00    0.00     0.00     0.00 4  186.9350000     -338000.000
    778.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          15600.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.176027770D+04-5.073431535D+01
Rb2O2(b)           Beta,rhombic Gurvich,1982 pt1 p433 pt2 p456.
 1 tpis82 RB  2.00O   2.00    0.00     0.00     0.00 1  202.9344000     -410000.000
    298.150    398.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19700.000
 0.000000000D+00 0.000000000D+00 2.566116344D+00 2.890861879D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.136136520D+04-3.996333599D+00
Rb2O2(a)           Alpha,cubic. Gurvich,1982 pt1 p433 pt2 p456.
 1 tpis82 RB  2.00O   2.00    0.00     0.00     0.00 2  202.9344000     -410000.000
    398.000    843.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19700.000
 0.000000000D+00 0.000000000D+00 1.407178535D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.365100100D+04-6.136883861D+01
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Rb2O2(L)            Liquid. Gurvich,1982 pt1 p433 pt2 p456.
 1 tpis82 RB  2.00O   2.00     0.00     0.00     0.00 3  202.9344000     -410000.000
    843.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          19700.000
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.284890920D+04-7.214727369D+01
Rb2SO4(a)           Alpha,rhombic. Gurvich,1982 pt1 p451 pt2 p475.
 3 tpis82 RB  2.00S   1.00O   4.00     0.00     0.00 1  266.9982000    -1435900.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27014.000
-1.192448350D+07 2.294293959D+05-1.785117228D+03 7.309062720D+00-1.617521748D-02
 1.861676545D-05-8.714648070D-09                 -1.202291196D+06 9.289553650D+03
    500.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27014.000
-4.871322610D+05 0.000000000D+00 2.853725036D+01-3.587804810D-02 4.220439770D-05
 0.000000000D+00 0.000000000D+00                 -1.816178572D+05-1.327574146D+02
    800.000    931.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27014.000
 0.000000000D+00 0.000000000D+00 3.464686434D+02-6.082068577D-01 0.000000000D+00
 3.246132364D-07 0.000000000D+00                 -2.782463487D+05-1.841656965D+03
Rb2SO4(b)           Beta,hexagonal. Gurvich,1982 pt1 p451 pt2 p475.
 1 tpis82 RB  2.00S   1.00O   4.00     0.00     0.00 2  266.9982000    -1435900.000
    931.000   1343.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27014.000
 0.000000000D+00 0.000000000D+00 1.107353290D+01 1.230667833D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.739435450D+05-3.919109508D+01
Rb2SO4(L)           Liquid. Gurvich,1982 pt1 p451 pt2 p475.
 1 tpis82 RB  2.00S   1.00O   4.00     0.00     0.00 3  266.9982000    -1435900.000
   1343.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          27014.000
 0.000000000D+00 0.000000000D+00 2.483609978D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.768420750D+05-1.184499504D+02
S(a)                Alpha. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
 1 tpis89 S   1.00    0.00     0.00     0.00     0.00 1   32.0650000          0.000
    200.000    368.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4412.000
-1.035710779D+04 0.000000000D+00 1.866766938D+00 4.256140250D-03-3.265252270D-06
 0.000000000D+00 0.000000000D+00                 -7.516389580D+02-7.961066980D+00
S(b)                Beta. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
 1 tpis89 S   1.00    0.00     0.00     0.00     0.00 2   32.0650000          0.000
    368.300    388.3607 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4412.000
 0.000000000D+00 0.000000000D+00 2.080514131D+00 2.440879557D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.852714730D+02-8.607846750D+00
S(L)                Liquid. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
 5 tpis89 S   1.00    0.00     0.00     0.00     0.00 3   32.0650000          0.000
    388.360    428.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4412.000
-6.366550765D+07 0.000000000D+00 2.376860693D+03-7.888076026D+00 7.376076522D-03
 0.000000000D+00 0.000000000D+00                 -6.356594920D+05-1.186929589D+04
    428.150    432.2507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4412.000
 0.000000000D+00 0.000000000D+00 6.928522306D+03-3.254655981D+01 3.824448176D-02
 0.000000000D+00 0.000000000D+00                 -9.832222680D+05-3.154806751D+04
    432.250    453.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4412.000
 0.000000000D+00 0.000000000D+00 1.649945697D+02-6.843534977D-01 7.315907973D-04
 0.000000000D+00 0.000000000D+00                 -2.638846929D+04-7.681730097D+02
    453.150    717.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4412.000
 1.972984578D+06 0.000000000D+00-2.441009753D+01 6.090352889D-02-3.744069103D-05
 0.000000000D+00 0.000000000D+00                  1.113013440D+04 1.363174183D+02
    717.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4412.000
 0.000000000D+00 0.000000000D+00 3.848693429D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -8.284589830D+02-1.736128237D+01
SCL2(L)             Chase,1998 p855.
 1 j 6/78 S   1.00CL  2.00     0.00     0.00     0.00 1  102.9710000     -49790.000
    298.150   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 1.094496248D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.251567000D+03-4.026872255D+01
S2CL2(L)            Chase,1998 p858.
 1 j 6/78 S   2.00CL  2.00     0.00     0.00     0.00 1  135.0360000     -58158.000
    298.150   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
 0.000000000D+00 0.000000000D+00 1.494856582D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.145167466D+04-5.824880790D+01
Sc(a)               Alpha. Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.
 2 tpis82 SC  1.00    0.00     0.00     0.00     0.00 1   44.9559100          0.000
    100.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5207.000
-5.723537690D+03 0.000000000D+00 1.835072325D+00 9.478861990D-03-2.317188582D-05
 2.004221829D-08 0.000000000D+00                 -8.225089040D+02-8.279121410D+00
    400.000   1609.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5207.000
-2.296409436D+04 0.000000000D+00 3.590296910D+00-1.480249906D-03 2.132230702D-06
-4.653598600D-10 0.000000000D+00                 -1.099543829D+03-1.605255360D+01
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Sc(b)              Beta. Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.
 1 tpis82 SC  1.00     0.00     0.00     0.00     0.00 2   44.9559100           0.000
   1609.000   1814.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           5207.000
 0.000000000D+00 0.000000000D+00 5.316007798D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.113439951D+03-2.875686543D+01
Sc(L)              Liquid. Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.
 1 tpis82 SC  1.00     0.00     0.00     0.00     0.00 3   44.9559100           0.000
   1814.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           5207.000
 0.000000000D+00 0.000000000D+00 5.291953464D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.373974847D+03-2.764152183D+01
Sc2O3(cr)          Cubic. Gurvich,1982 pt1 p145 pt2 p150.
 2 tpis82 SC  2.000    3.00     0.00     0.00     0.00 1  137.9100200   -1908600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13930.000
-2.372563268D+06 4.573798990D+04-3.655376590D+02 1.588230977D+00-3.584389210D-03
 4.185870320D-06-1.985472581D-09                 -4.353786390D+05 1.884709407D+03
    500.000   2762.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13930.000
-2.669869135D+05 0.000000000D+00 1.386002327D+01 1.535415402D-03 1.928963573D-07
 0.000000000D+00 0.000000000D+00                 -2.346482672D+05-7.170005710D+01
Sc2O3(L)           Liquid. Gurvich,1982 pt1 p145 pt2 p150.
 1 tpis82 SC  2.000    3.00     0.00     0.00     0.00 2  137.9100200   -1908600.000
   2762.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           13930.000
 0.000000000D+00 0.000000000D+00 2.405433393D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.402224225D+05-1.419525042D+02
Si(cr)             Cubic. Ref-Elm. Gurvich,1991 pt1 p236 pt2 p220.
 2 tpis91 SI  1.00     0.00     0.00     0.00     0.00 1   28.0855000           0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           3217.471
-2.323538208D+04 0.000000000D+00 2.102021680D+00 1.809220552D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.850635210D+02-1.038427318D+01
    298.150   1690.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           3217.471
-5.232559740D+04 0.000000000D+00 2.850169415D+00 3.975166970D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.042947234D+03-1.438964187D+01
Si(L)              Liquid. Ref-Elm. Gurvich,1991 pt1 p236 pt2 p220.
 1 tpis91 SI  1.00     0.00     0.00     0.00     0.00 2   28.0855000           0.000
   1690.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           3217.471
 0.000000000D+00 0.000000000D+00 3.271389414D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 4.882667110D+03-1.326611073D+01
SiC(b)             Beta,cubic. Gurvich,1991 pt1 p298 pt2 p264.
 2 tpis91 SI  1.00C    1.00     0.00     0.00     0.00 1   40.0962000      -73000.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           3272.000
-2.285496383D+03 0.000000000D+00-5.349100620D-01 1.271547084D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.193174900D+03 1.241441354D+00
    298.150   3105.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           3272.000
-1.269106658D+05 0.000000000D+00 3.757286960D+00 3.481744565D-03-1.620660748D-06
 2.611097948D-10 0.000000000D+00                 -1.046667760D+04-2.109198538D+01
SiC(L)             Liquid. Gurvich,1991 pt1 p298 pt2 p264.
 1 tpis91 SI  1.00C    1.00     0.00     0.00     0.00 2   40.0962000      -73000.000
   3103.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           3272.000
 0.000000000D+00 0.000000000D+00 7.577115188D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.787459000D+03-4.367596159D+01
SiO2(a-qz)         Alpha-quartz,hexagonal. Gurvich,1991 pt1 p250 pt2 p228.
 1 tpis91 SI  1.00O    2.00     0.00     0.00     0.00 1   60.0843000     -910700.000
    200.000    848.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6916.000
-5.776895500D+05 7.214661110D+03-3.145730294D+01 7.412177150D-02-8.670077820D-06
-1.080461312D-07 8.316324910D-11                -1.462398375D+05 1.842424399D+02
SiO2(b-qz)         Beta-quartz,hexagonal. Gurvich,1991 pt1 p250 pt2 p228.
 1 tpis91 SI  1.00O    2.00     0.00     0.00     0.00 2   60.0843000     -910700.000
    848.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6916.000
 2.317635074D+04 0.000000000D+00 7.026511484D+00 1.241925261D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.117012474D+05-3.580751356D+01
SiO2(b-crt)        Beta-cristobalite,cubic. Gurvich,1991 pt1 p250 pt2 p228.
 1 tpis91 SI  1.00O    2.00     0.00     0.00     0.00 3   60.0843000     -910700.000
   1200.000   1996.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6916.000
-5.356419079D+05 0.000000000D+00 9.331036946D+00-7.306503931D-04 3.339944266D-07
 0.000000000D+00 0.000000000D+00                 -1.134326721D+05-4.998768383D+01
SiO2(L)            Liquid. Gurvich,1991 pt1 p250 pt2 p228.
 1 tpis91 SI  1.00O    2.00     0.00     0.00     0.00 4   60.0843000     -910700.000
   1996.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6916.000
 0.000000000D+00 0.000000000D+00 1.004268442D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.140002976D+05-5.554279592D+01
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SiS(cr)             Crystal. Gurvich,1991 pt1 p289 pt2 p257.
 1 tpis91 SI  1.00S   1.00    0.00    0.00    0.00 1   60.1505000     -168737.210
    298.150   1363.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9000.490
 0.000000000D+00 0.000000000D+00 4.873408054D+00 1.807202108D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.182763678D+04-2.072841584D+01
SiS(L)              Liquid. Gurvich,1991 pt1 p289 pt2 p257.
 1 tpis91 SI  1.00S   1.00    0.00    0.00    0.00 2   60.1505000     -168737.210
   1363.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9000.490
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.076140696D+04-3.851581605D+01
SiS2(cr)            Tetragonal. Gurvich,1991 pt1 p293 pt2 p259.
 2 tpis91 SI  1.00S   2.00    0.00    0.00    0.00 1   92.2155000     -287000.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11180.490
-1.489679569D+04 0.000000000D+00 3.921710460D+00 1.226970632D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.628253940D+04-1.684224727D+01
    298.150   1363.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11180.490
 0.000000000D+00 0.000000000D+00 6.423349061D+00 3.317212921D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.658052990D+04-2.834259902D+01
SiS2(L)             Liquid. Gurvich,1991 pt1 p293 pt2 p259.
 1 tpis91 SI  1.00S   2.00    0.00    0.00    0.00 2   92.2155000     -287000.000
   1363.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11180.490
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.909260770D+04-6.276638967D+01
Si2N2O(cr)          Fegley,1981.
 2 g 7/95 SI  2.00N   2.00O   1.00    0.00    0.00 1  100.1838000     -947700.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-7.783293180D+06 7.787697680D+04-3.226727260D+02 7.513788890D-01-9.139450720D-04
 5.774402010D-07-1.479973902D-10                -5.139865410D+05 1.873124449D+03
   1000.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-7.414096340D+06 2.559424417D+04-2.535540920D+01 3.208894230D-02-1.340182230D-05
 3.075006784D-09-2.892800339D-13                -2.762647725D+05 1.907774092D+02
Si3N4(cr)           Hexagonal. Gurvich,1991 pt1 p297 pt2 p262.
 2 tpis91 SI  3.00N   4.00    0.00    0.00    0.00 1  140.2833000     -787800.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12113.490
-1.136434515D+04 0.000000000D+00-4.993435710D-01 3.962318940D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.640037870D+04-1.086768954D+00
    298.150   4000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12113.490
-2.910454134D+05 0.000000000D+00 1.189210188D+01 9.349799327D-03-2.551082385D-06
 2.857654871D-10 0.000000000D+00                -9.966541740D+04-6.412447976D+01
Sn(cr)              CrI,tetragonal. Ref-Elm. Gurvich,1991 pt1 p350 pt2 p300.
 1 tpis91 SN  1.00    0.00    0.00    0.00    0.00 1  118.7100000           0.000
    200.000    505.1187 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6323.000
-9.970568110D+05 1.865056292D+04-1.393005103D+02 5.652800870D-01-1.229162587D-03
 1.398259924D-06-6.465843270D-10                -8.479846440D+04 7.317981190D+02
Sn(L)               Liquid. Ref-Elm. Gurvich,1991 pt1 p350 pt2 p300.
 1 tpis91 SN  1.00    0.00    0.00    0.00    0.00 2  118.7100000           0.000
    505.118   4700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6323.000
 9.847844311D+04 0.000000000D+00 3.028921728D+00 2.531718646D-04-1.960428215D-08
 0.000000000D+00 0.000000000D+00                 2.209652103D+02-9.089783541D+00
SnBr2(cr)           Rhombic. Gurvich,1991 pt1 p379 pt2 p322.
 2 tpis91 SN  1.00BR  2.00    0.00    0.00    0.00 1  278.5180000     -253600.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18670.000
-1.072142073D+04 0.000000000D+00 8.650388720D+00 3.246938990D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.326028440D+04-3.191324070D+01
    298.150    503.4007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18670.000
 1.596365871D+05 0.000000000D+00 4.310656912D+00 1.137469316D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.175626170D+04-8.652273965D+00
SnBr2(L)            Liquid. Gurvich,1991 pt1 p379 pt2 p322.
 2 tpis91 SN  1.00BR  2.00    0.00    0.00    0.00 2  278.5180000     -253600.000
    503.400    860.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18670.000
 2.804494793D+05 0.000000000D+00 1.427732963D+01-2.218170403D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.305162210D+04-6.008238208D+01
    860.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18670.000
 0.000000000D+00 0.000000000D+00 1.274879698D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.288346740D+04-5.185141223D+01
SnBr4(cr)           Monoclinic. Gurvich,1991 pt1 p382 pt2 p325.
 1 tpis91 SN  1.00BR  4.00    0.00    0.00    0.00 1  438.3260000     -388000.000
    200.000    302.2507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         31260.000
-3.870038960D+06 0.000000000D+00 3.663330300D+02-1.775658617D+00 2.504656832D-03
 0.000000000D+00 0.000000000D+00                -1.120730416D+05-1.659626236D+03
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SnBr4(L)          Liquid. Gurvich,1991 pt1 p382 pt2 p325.
 2 tpis91 SN  1.00BR  4.00     0.00     0.00     0.00 2  438.3260000     -388000.000
    302.250    470.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31260.000
 1.124780655D+05 0.000000000D+00 1.859869072D+01-4.792826035D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.036569340D+04-6.913668591D+01
    470.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31260.000
 0.000000000D+00 0.000000000D+00 1.888265213D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.079140710D+04-7.136367786D+01
SnCL2(cr)         Rhombic. Gurvich,1991 pt1 p372 pt2 p316.
 1 tpis91 SN  1.00CL  2.00     0.00     0.00     0.00 1  189.6160000     -333000.000
    200.000    520.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17330.000
-3.455659100D+05 5.121048940D+03-2.179939832D+01 8.738265750D-02-1.087380837D-04
 5.701191040D-08 0.000000000D+00                 -6.692353080D+04 1.338412221D+02
SnCL2(L)          Liquid. Gurvich,1991 pt1 p372 pt2 p316.
 1 tpis91 SN  1.00CL  2.00     0.00     0.00     0.00 2  189.6160000     -333000.000
    520.200   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          17330.000
 0.000000000D+00 0.000000000D+00 1.322988366D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.294240400D+04-5.766924967D+01
SnCL4(L)          Liquid. Gurvich,1991 pt1 p375 pt2 p319.
 2 tpis91 SN  1.00CL  4.00     0.00     0.00     0.00 1  260.5220000     -517000.000
    239.050    350.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          38740.000
 0.000000000D+00 0.000000000D+00 2.059050984D+01-5.567014773D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.807207820D+04-8.378462335D+01
    350.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          38740.000
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -6.773111750D+04-7.431947542D+01
SnF2(cr)          Monoclinic. Gurvich,1991 pt1 p367 pt2 p311.
 1 tpis91 SN  1.00F   2.00     0.00     0.00     0.00 1  156.7068064     -677000.000
    298.150    488.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14200.000
 0.000000000D+00 0.000000000D+00 6.575252180D+00 7.150150760D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -8.370213250D+04-2.802481800D+01
SnF2(L)           Liquid. Gurvich,1991 pt1 p367 pt2 p311.
 1 tpis91 SN  1.00F   2.00     0.00     0.00     0.00 2  156.7068064     -677000.000
    488.200   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14200.000
 0.000000000D+00 0.000000000D+00 1.202716700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -8.424882400D+04-5.569866810D+01
SnI2(cr)          Monoclinic. Gurvich,1991 pt1 p386 pt2 p328.
 1 tpis91 SN  1.00I   2.00     0.00     0.00     0.00 1  372.5189400     -153000.000
    200.000    595.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18950.000
 8.194427570D+05-1.285027272D+04 8.314392190D+01-1.959449848D-01 2.384765022D-04
-9.891789320D-08 0.000000000D+00                 3.957086730D+04-4.432502620D+02
SnI2(L)           Liquid. Gurvich,1991 pt1 p386 pt2 p328.
 2 tpis91 SN  1.00I   2.00     0.00     0.00     0.00 2  372.5189400     -153000.000
    595.700    960.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18950.000
 3.807680789D+05 0.000000000D+00 1.313799611D+01-7.105650243D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.013964325D+04-5.193401798D+01
    960.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18950.000
 0.000000000D+00 0.000000000D+00 1.286906865D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.060553468D+04-5.097603343D+01
SnI4(cr)          Cubic. Gurvich,1991 pt1 p389 pt2 p331
 1 tpis91 SN  1.00I   4.00     0.00     0.00     0.00 1  626.3278800     -207500.000
    200.000    418.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31600.000
 1.365815960D+06-2.186441599D+04 1.411768692D+02-3.151970333D-01 2.991203201D-04
 0.000000000D+00 0.000000000D+00                 7.347422460D+04-7.553382720D+02
SnI4(L)           Liquid. Gurvich,1991 pt1 p389 pt2 p331
 2 tpis91 SN  1.00I   4.00     0.00     0.00     0.00 2  626.3278800     -207500.000
    418.000    580.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31600.000
 3.125499879D+05 0.000000000D+00 2.114568387D+01-5.918328320D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.828678876D+04-7.927900653D+01
    580.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          31600.000
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.836905732D+04-6.724586950D+01
SnO(cr)           Tetragonal. Gurvich,1991 pt1 p356 pt2 p306.
 2 tpis91 SN  1.00O   1.00     0.00     0.00     0.00 1  134.7094000     -280710.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8736.000
 0.000000000D+00 0.000000000D+00 7.279467580D-02 3.307685420D-02-4.710942000D-05
 0.000000000D+00 0.000000000D+00                 -3.483713220D+04-1.306828645D+00
    298.150   1250.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8736.000
 0.000000000D+00 0.000000000D+00 5.260682830D+00 1.630883840D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.540242040D+04-2.358356588D+01
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SnO(L)              Liquid. Gurvich,1991 pt1 p356 pt2 p306.
 1 tpis91 SN  1.00O   1.00     0.00     0.00     0.00 2  134.7094000     -280710.000
   1250.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8736.000
 0.000000000D+00 0.000000000D+00 7.577115188D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.369230760D+04-3.539798567D+01
SnO2(cr)            Tetragonal. Gurvich,1991 pt1 p361 pt2 p308.
 2 tpis91 SN  1.00O   2.00     0.00     0.00     0.00 1  150.7088000     -577630.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8384.000
 0.000000000D+00 0.000000000D+00-1.177647966D+00 3.970167880D-02-4.790758920D-05
 0.000000000D+00 0.000000000D+00                 -7.046277710D+04 2.896556966D+00
    298.150   1903.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8384.000
-2.674601390D+05 0.000000000D+00 9.145457760D+00 8.856805753D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.313567410D+04-4.798106778D+01
SnO2(L)             Liquid. Gurvich,1991 pt1 p361 pt2 p308.
 1 tpis91 SN  1.00O   2.00     0.00     0.00     0.00 2  150.7088000     -577630.000
   1903.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8384.000
 0.000000000D+00 0.000000000D+00 1.106499361D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.222994130D+04-5.927455845D+01
SnS(cr)             Rhombic. Gurvich,1991 pt1 p392 pt2 p333.
 2 tpis91 SN  1.00S   1.00     0.00     0.00     0.00 1  150.7750000     -109662.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10530.000
-1.473490121D+04 0.000000000D+00 5.317316410D+00 2.586688381D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.493898062D+04-2.188910671D+01
    298.150    875.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10530.000
 3.056103126D+04 0.000000000D+00 4.511751143D+00 3.579405160D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.459100103D+04-1.734052255D+01
SnS(cr)             Cubic. Gurvich,1991 pt1 p392 pt2 p333.
 1 tpis91 SN  1.00S   1.00     0.00     0.00     0.00 2  150.7750000     -109662.000
    875.000   1154.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10530.000
 0.000000000D+00 0.000000000D+00 4.921516722D+00 1.882251630D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.425419920D+04-1.855922147D+01
SnS(L)              Liquid. Gurvich,1991 pt1 p392 pt2 p333.
 1 tpis91 SN  1.00S   1.00     0.00     0.00     0.00 3  150.7750000     -109662.000
   1154.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          10530.000
 0.000000000D+00 0.000000000D+00 9.008348057D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.391650549D+04-4.190990669D+01
SnS2(cr)            Hexagonal. Gurvich,1991 pt1 p396 pt2 p335.
 2 tpis91 SN  1.00S   2.00     0.00     0.00     0.00 1  182.8400000     -141837.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13310.000
-2.817980768D+04 0.000000000D+00 6.586339710D+00 7.259692260D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.943987500D+04-2.933754416D+01
    298.150   1143.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          13310.000
 1.193094963D+04 0.000000000D+00 7.560277154D+00 2.479641013D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.938326475D+04-3.323586315D+01
Sr(a)               Alpha. Ref-Elm. Alcock,1993.
 2 srd 93 SR  1.00    0.00     0.00     0.00     0.00 1   87.6200000          0.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6558.289
-4.150245670D+03 1.559823384D+02-2.623173257D-01 2.945369354D-02-1.212940361D-04
 2.401045642D-07-1.708772572D-10                 -1.455791066D+03 3.435106060D+00
    298.150    820.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6558.289
 1.294412876D+05-1.646179180D+03 1.111114164D+01-1.973737192D-02 2.910871519D-05
-2.163423606D-08 6.508160860D-12                 7.160398040D+03-5.671602200D+01
Sr(b)               Beta. Ref-Elm. Alcock,1993.
 1 srd 93 SR  1.00    0.00     0.00     0.00     0.00 2   87.6200000          0.000
    820.000   1041.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6558.289
 0.000000000D+00 0.000000000D+00 3.190326309D+00 4.837326553D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -8.560991280D+02-1.157238431D+01
Sr(L)               Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 SR  1.00    0.00     0.00     0.00     0.00 3   87.6200000          0.000
   1041.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6558.289
 0.000000000D+00 0.000000000D+00 4.450051777D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -9.431940390D+02-1.889703393D+01
SrBr2(a)            Alpha,tetragonal. Gurvich,1996a pt1 p523 pt2 p403.
 1 tpis96 SR  1.00BR  2.00     0.00     0.00     0.00 1  247.4280000     -722000.000
    200.000    918.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18060.499
-1.563862878D+05 2.048387286D+03-2.389924996D+00 3.200996340D-02-4.324517230D-05
 3.247344210D-08-9.786717550D-12                 -9.941922340D+04 2.897007516D+01
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SrBr2(b)          Beta. Gurvich,1996a pt1 p523 pt2 p403.
 1 tpis96 SR  1.00BR  2.00    0.00    0.00    0.00 2  247.4280000    -722000.000
    918.000    930.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18060.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.021650510D+04-5.212663905D+01
SrBr2(L)          Liquid. Gurvich,1996a pt1 p523 pt2 p403.
 1 tpis96 SR  1.00BR  2.00    0.00    0.00    0.00 3  247.4280000    -722000.000
    930.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18060.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.900176120D+04-5.082046285D+01
SrCO3(a)          Alpha,rhombic. Gurvich,1996a pt1 p532 pt2 p411.
 2 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 1  147.6289000   -1226000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15120.499
-3.185109310D+07 5.983944250D+05-4.555778730D+03 1.807422903D+01-3.922550990D-02
 4.443338240D-05-2.057838162D-08                -2.840270234D+06 2.379927032D+04
    500.000   1198.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15120.499
-4.737741611D+05 0.000000000D+00 1.829247905D+01-1.342833192D-02 1.073412624D-05
 0.000000000D+00 0.000000000D+00                -1.539939771D+05-9.167197246D+01
SrCO3(b)          Beta,rhombic. Gurvich,1996a pt1 p532 pt2 p411.
 1 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 2  147.6289000   -1226000.000
   1198.000   1689.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15120.499
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.541962605D+05-9.302015968D+01
SrCO3(c)          Gamma,cubic. Gurvich,1996a pt1 p532 pt2 p411.
 1 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 3  147.6289000   -1226000.000
   1689.000   1767.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15120.499
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.541962605D+05-9.302015968D+01
SrCO3(L)          Liquid. Gurvich,1996a pt1 p532 pt2 p411.
 1 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 4  147.6289000   -1226000.000
   1767.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15120.499
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.534232745D+05-1.073837834D+02
SrCL2(a)          Alpha,cubic. Gurvich,1996a pt1 p518 pt2 p400.
 2 tpis96 SR  1.00CL  2.00    0.00    0.00    0.00 1  158.5260000    -833000.000
    200.000    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16230.000
-8.219302560D+05 1.414627236D+04-9.066868860D+01 3.537351300D-01-6.601840230D-04
 6.294183590D-07-2.405335168D-10                -1.675299882D+05 4.920219760D+02
    700.000    990.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16230.000
 1.112527665D+09 0.000000000D+00-1.718772952D+04 4.254819093D+01-3.935556431D-02
 1.290928281D-05 0.000000000D+00                6.824931370D+06 9.213791630D+04
SrCL2(b)          Beta,cubic. Gurvich,1996a pt1 p518 pt2 p400.
 1 tpis96 SR  1.00CL  2.00    0.00    0.00    0.00 2  158.5260000    -833000.000
    900.000   1147.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16230.000
 2.652616089D+08 0.000000000D+00-6.137593196D+02 3.705888862D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                6.013938810D+05 4.028366895D+03
SrCL2(L)          Liquid. Gurvich,1996a pt1 p518 pt2 p400.
 1 tpis96 SR  1.00CL  2.00    0.00    0.00    0.00 3  158.5260000    -833000.000
   1147.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16230.000
-1.621863465D+06 0.000000000D+00 1.278463794D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.040518221D+05-6.010500872D+01
SrF2(a)           Alpha,cubic. Gurvich,1996a pt1 p513 pt2 p396.
 2 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 1  125.6168064   -1229000.000
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13075.000
-1.436181472D+04-3.902704550D+02 9.084528850D+00 4.747017010D-03-9.922331280D-06
 1.169135473D-08-4.825603120D-12                -1.484911532D+05-4.433988680D+01
    800.000   1484.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13075.000
-1.706744719D+07 2.576630531D+04 3.257893350D+01-3.032276697D-02-2.832102640D-05
 2.982419101D-08-2.378577761D-12                -3.511043830D+05-1.514196992D+02
SrF2(b)           Beta,cubic. Gurvich,1996a pt1 p513 pt2 p396.
 1 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 2  125.6168064   -1229000.000
   1484.000   1750.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13075.000
 5.274154560D+09-9.287005960D+04-1.188369557D+04 9.829240680D+00-2.277347958D-03
 0.000000000D+00 0.000000000D+00                1.339064905D+07 7.586298750D+04
SrF2(L)           Liquid. Gurvich,1996a pt1 p515 pt2 p396.
 1 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 3  125.6168064   -1229000.000
   1750.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13075.000
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.478877648D+05-5.796718683D+01
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SrH2(a)           Alpha,rhombic. Gurvich,1996a pt1 p501 pt2 p389.
 1 tpis96 SR  1.00H   2.00    0.00    0.00    0.00 1   89.6358800    -180000.000
    298.000   1128.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8000.499
 0.000000000D+00 0.000000000D+00 4.125438541D+00 3.912437414D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.305279501D+04-1.841745147D+01
SrH2(b)           Beta. Gurvich,1996a pt1 p501 pt2 p389.
 1 tpis96 SR  1.00H   2.00    0.00    0.00    0.00 2   89.6358800    -180000.000
   1128.000   1323.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8000.499
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.467660041D+04-4.425795748D+01
SrH2(L)           Liquid. Gurvich,1996a pt1 p501 pt2 p389.
 1 tpis96 SR  1.00H   2.00    0.00    0.00    0.00 3   89.6358800    -180000.000
   1323.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8000.499
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.254682969D+04-4.562495289D+01
SrI2(cr)          Rhombic. Gurvich,1996a pt1 p527 pt2 p406.
 1 tpis96 SR  1.00I   2.00    0.00    0.00    0.00 1  341.4289400    -568000.000
    200.000    811.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18920.499
-8.531836590D+05 1.396294943D+04-8.134381170D+01 2.923620048D-01-4.941293260D-04
 4.280629170D-07-1.479234641D-10                -1.358835709D+05 4.559376890D+02
SrI2(L)           Liquid. Gurvich,1996a pt1 p527 pt2 p406.
 1 tpis96 SR  1.00I   2.00    0.00    0.00    0.00 2  341.4289400    -568000.000
    811.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18920.499
 0.000000000D+00 0.000000000D+00 1.322988366D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.143040870D+04-5.646969655D+01
SrO(cr)           Cubic. Gurvich,1996a pt1 p494 pt2 p383.
 3 tpis96 SR  1.00O   1.00    0.00    0.00    0.00 1  103.6194000    -591000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.499
-1.625438799D+06 2.932375088D+04-2.136643281D+02 8.526581540D-01-1.819594223D-03
 2.035599655D-06-9.340883290D-10                -2.053069998D+05 1.123784285D+03
    500.000   1800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.499
-3.410904551D+04 0.000000000D+00 5.049245235D+00 3.431471007D-03-3.042151612D-06
 9.069686608D-10 0.000000000D+00                -7.282782040D+04-2.317163697D+01
   1800.000   2805.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.499
-3.971117961D+07 0.000000000D+00 7.850733236D+01-5.336790743D-02 1.125297823D-05
 0.000000000D+00 0.000000000D+00                -1.604896850D+05-4.990588969D+02
SrO(L)            Liquid. Gurvich,1996a pt1 p494 pt2 p383.
 1 tpis96 SR  1.00O   1.00    0.00    0.00    0.00 2  103.6194000    -591000.000
   2805.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.499
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.188203330D+04-5.541556063D+01
Sr(OH)2(b)        Beta,tetragonal. Gurvich,1996a pt1 p505 pt2 p392.
 1 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 1  121.6346800    -964300.000
    200.000    753.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15272.499
 5.749774650D+05-9.564782420D+03 6.310466570D+01-1.470270543D-01 2.468488663D-04
-2.041763520D-07 6.865596260D-11                -7.364279180D+04-3.424340180D+02
Sr(OH)2(a)        Alpha. Gurvich,1996a pt1 p505 pt2 p392.
 1 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 2  121.6346800    -964300.000
    753.000    808.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15272.499
 0.000000000D+00 0.000000000D+00 1.563531705D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.216576455D+05-8.006737394D+01
Sr(OH)2(L)        Liquid. Gurvich,1996a pt1 p505 pt2 p392.
 1 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 3  121.6346800    -964300.000
    808.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         15272.499
 0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.211265258D+05-9.516262078D+01
SrS(cr)           Cubic. Gurvich,1996a pt1 p528 pt2 p408.
 2 tpis96 SR  1.00S   1.00    0.00    0.00    0.00 1  119.6850000    -480000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10040.499
 2.688173776D+06-5.010846740D+04 3.813026790D+02-1.462623236D+00 3.138875273D-03
-3.522660370D-06 1.619531388D-09                1.665724752D+05-1.992760719D+03
    500.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10040.499
-1.221960164D+04 0.000000000D+00 5.716873273D+00 9.316243531D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.951728090D+04-2.471633956D+01
SrS(L)            Liquid. Gurvich,1996a pt1 p528 pt2 p408.
 1 tpis96 SR  1.00S   1.00    0.00    0.00    0.00 2  119.6850000    -480000.000
   2500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         10040.499
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.487727330D+04-3.767411768D+01
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SrS04(a)          Alpha,Rhombic. Gurvich,1996a pt1 p531 pt2 p410.
 1 tpis96 SR  1.00S   1.00O   4.00     0.00     0.00 1  183.6826000   -1457000.000
    298.150   1430.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18400.499
-2.524863161D+05 0.000000000D+00 1.319271972D+01 6.424070691D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.803016041D+05-6.394942426D+01
SrS04(b)          Beta,hexagonal. Gurvich,1996a pt1 p531 pt2 p410.
 1 tpis96 SR  1.00S   1.00O   4.00     0.00     0.00 2  183.6826000   -1457000.000
   1430.000   1880.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18400.499
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.827264862D+05-1.065597408D+02
SrS04(L)          Liquid. Gurvich,1996a pt1 p531 pt2 p410.
 1 tpis96 SR  1.00S   1.00O   4.00     0.00     0.00 3  183.6826000   -1457000.000
   1880.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18400.499
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.783967061D+05-1.042566663D+02
Ta(cr)            Crystal. Ref-Elm. Chase,1998 pp1899-1901.
 3 j12/72 TA  1.00    0.00     0.00     0.00     0.00 1  180.9479000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5681.000
 1.519941999D+04-4.927143830D+02 6.855605760D+00-1.366625579D-02 2.561466303D-05
-2.235631116D-08 7.389831320D-12                 1.236077891D+03-3.252075490D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5681.000
-1.002219854D+08 4.696591430D+05-8.992639340D+02 9.084714280D-01-5.043323480D-04
 1.463919859D-07-1.734426993D-11                 -2.762235634D+06 5.939534460D+03
   2000.000   3258.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5681.000
 3.305034810D+05 8.564351680D+01-1.797593491D+00 6.549784340D-03-2.878793550D-06
 4.952725110D-10-7.703452530D-15                 1.556933077D+03 1.641047132D+01
Ta(L)             Liquid. Ref-Elm. Chase,1998 pp1899-1901.
 1 j12/72 TA  1.00    0.00     0.00     0.00     0.00 2  180.9479000          0.000
   3258.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5681.000
 0.000000000D+00 0.000000000D+00 5.032166658D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.436042760D+02-2.597362534D+01
TaC(cr)           Chase,1998 pp652-4.
 2 j12/73 TA  1.00C   1.00     0.00     0.00     0.00 1  192.9586000    -144096.960
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6514.488
-1.182153887D+04 2.152843262D+02-1.710781252D+00 3.226351270D-02-6.059170690D-05
 5.540177420D-08-1.961814434D-11                 -1.908587628D+04 8.122034510D+00
    800.000   4273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6514.488
-1.540090534D+05 2.156690707D+02 5.001633620D+00 1.161840292D-03-1.062186764D-07
 2.082367078D-11-1.580991193D-15                 -2.062101769D+04-2.388952788D+01
TaC(L)            Chase,1998 pp652-4.
 1 j12/73 TA  1.00C   1.00     0.00     0.00     0.00 2  192.9586000    -144096.960
   4273.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6514.488
 0.000000000D+00 0.000000000D+00 8.051466653D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.010399602D+04-4.208381497D+01
Ta2O5(II)         Rhombic. Gurvich,1982 pt1 p91 pt2 p92.
 2 tpis82 TA  2.00O   5.00     0.00     0.00     0.00 1  441.8928000   -2049000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22950.000
-3.279677980D+06 6.126833460D+04-4.710233330D+02 1.998455231D+00-4.425553760D-03
 5.098341430D-06-2.392974558D-09                 -5.247547580D+05 2.448363106D+03
    500.000   1633.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22950.000
-2.735481912D+05 0.000000000D+00 1.819193368D+01 3.735655440D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.529440756D+05-8.923622860D+01
Ta2O5(I)          Monoclinic. Gurvich,1982 pt1 p91 pt2 p92.
 1 tpis82 TA  2.00O   5.00     0.00     0.00     0.00 2  441.8928000   -2049000.000
   1633.000   2150.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22950.000
 0.000000000D+00 0.000000000D+00 2.525705063D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.590924400D+05-1.352062771D+02
Ta2O5(L)          Liquid. Gurvich,1982 pt1 p91 pt2 p92.
 1 tpis82 TA  2.00O   5.00     0.00     0.00     0.00 3  441.8928000   -2049000.000
   2150.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22950.000
 0.000000000D+00 0.000000000D+00 2.645976732D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.472456805D+05-1.377221533D+02
Th(a)             Alpha. Ref-Elm. Cox,1989 p239.
 1 coda89 TH  1.00    0.00     0.00     0.00     0.00 1  232.0381000          0.000
    200.000   1650.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6350.000
-1.453247151D+04 1.505222433D+02 2.270694767D+00 2.058614354D-03-9.216614670D-07
 4.316796340D-10-7.950656800D-14                 -1.667536353D+03-6.857176980D+00
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Th(b)              Beta. Ref-Elm. Cox,1989 p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 2  232.0381000          0.000
   1650.000   2023.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6350.000
 8.360316570D+06-2.333327743D+04 2.783594798D+01-1.293559561D-02 3.966098040D-06
-4.361984440D-10 0.000000000D+00                 1.501326293D+05-1.894583434D+02
Th(L)              Liquid. Ref-Elm. Cox,1989 p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 3  232.0381000          0.000
   2023.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6350.000
 0.000000000D+00 0.000000000D+00 5.532496804D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.191824935D+03-2.760071917D+01
Ti(a)              Alpha. Ref-Elm. Cox,1989 p230.
 2 coda89 TI  1.00    0.00    0.00    0.00    0.00 1   47.8670000          0.000
    200.000    900.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4824.000
 3.598601350D+04-8.272305960D+02 7.689097770D+00-1.143968449D-02 1.392105464D-05
-4.691057160D-09-9.852130400D-13                 2.936621421D+03-3.985138010D+01
    900.000   1156.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4824.000
-2.876235910D+06 0.000000000D+00 4.573153420D+01-7.692381600D-02 3.799919490D-05
 0.000000000D+00 0.000000000D+00                -2.038023972D+04-2.516270281D+02
Ti(b)              Beta. Ref-Elm. Cox,1989 p230.
 1 coda89 TI  1.00    0.00    0.00    0.00    0.00 2   47.8670000          0.000
   1156.000   1944.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4824.000
-1.698740574D+06 6.576601240D+03-8.556182950D+00 9.789585830D-03-3.992418760D-06
 1.123642773D-09-1.201048055D-13                -3.929918290D+04 6.506590190D+01
Ti(L)              Liquid. Ref-Elm. Cox,1989 p230.
 1 coda89 TI  1.00    0.00    0.00    0.00    0.00 3   47.8670000          0.000
   1944.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4824.000
 0.000000000D+00 0.000000000D+00 5.628714139D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.377354619D+03-3.079443471D+01
TiB(cr)            Crystal. Chase,1998. p258.
 2 j 6/65 TI  1.00B   1.00    0.00    0.00    0.00 1   58.6780000    -160247.000
    298.150   1100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 5.892962460D+05-7.628387170D+03 3.264504220D+01-4.438679670D-02 4.037756110D-05
-1.901806786D-08 3.662438970D-12                 1.808566462D+04-1.924926707D+02
   1100.000   4000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 9.736238960D+05-2.744306202D+03 9.195602010D+00-1.636706129D-03 5.676930840D-07
-9.258425040D-11 6.105669480D-15                -3.925082340D+03-5.367424570D+01
TiB2(cr)           Crystal. Chase,1998 pp276-8.
 2 j 6/65 TI  1.00B   2.00    0.00    0.00    0.00 1   69.4890000    -279491.000
    200.000   2300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             5577.000
 2.701885716D+05-3.989107020D+03 1.904595810D+01-1.467951261D-02 1.249126541D-05
-4.481179720D-09 5.932523160D-13                -1.510818691D+04-1.130901290D+02
   2300.000   3193.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             5577.000
 2.449855642D+10-5.420046130D+07 4.984385950D+04-2.437314870D+01 6.688502930D-03
-9.763538800D-07 5.923249200D-11                 3.589528270D+08-3.651406280D+05
TiB2(L)            Liquid. Chase,1998 pp276-8.
 1 j 6/65 TI  1.00B   2.00    0.00    0.00    0.00 2   69.4890000    -279491.000
   3193.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             5577.000
 0.000000000D+00 0.000000000D+00 1.308363331D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.298172270D+04-7.649131141D+01
TiC(cr)            Chase,1998 p655-7
 2 j 6/68 TI  1.00C   1.00    0.00    0.00    0.00 1   59.8777000    -184096.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             4606.584
-2.936209453D+05 4.040416860D+03-2.309999326D+01 8.695403030D-02-1.254447445D-04
 8.803423830D-08-2.403516957D-11                -4.217890880D+04 1.253486677D+02
   1000.000   3290.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             4606.584
-3.586824960D+05 1.130360992D+03 4.571181220D+00 4.332844010D-04 4.730133770D-07
-1.025727737D-10 8.572441560D-15                -3.129994969D+04-2.180975207D+01
TiC(L)             Chase,1998 p655-7
 1 j 6/68 TI  1.00C   1.00    0.00    0.00    0.00 2   59.8777000    -184096.000
   3290.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             4606.584
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.766010062D+04-4.062778302D+01
TiCL2(cr)          Chase,1998 p865.
 2 j12/68 TI  1.00CL  2.00    0.00    0.00    0.00 1  118.7730000    -515470.000
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            13300.936
 6.275502170D+05-1.149039253D+04 8.470916630D+01-2.539508065D-01 4.582690050D-04
-4.167293950D-07 1.508542615D-10                -1.168917881D+04-4.484122170D+02
    800.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            13300.936
 3.621030580D+06-1.684661798D+04 4.010076440D+01-2.963515568D-02 1.756075169D-05
-5.065847400D-09 5.988802280D-13                 3.466967030D+04-2.478759697D+02
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TiCL3(cr)          Chase,1998 p886.
 1 j12/68 TI  1.00CL  3.00    0.00    0.00    0.00 1  154.2260000    -721740.000
    298.150   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         20920.000
 1.457928527D+05-1.355589207D+03 1.563840194D+01-4.771661650D-03 4.776265870D-06
-1.901286451D-09 3.011222662D-13                -8.308136940D+04-7.479338350D+01
TiCL4(L)           Chase,1998 p904.
 2 j12/67 TI  1.00CL  4.00    0.00    0.00    0.00 1  189.6790000    -804164.800
    249.046    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26963.000
 1.179781205D+06-1.710994382D+04 1.180652525D+02-3.089428313D-01 5.234695800D-04
-4.608788890D-07 1.654264781D-10                -2.053742284D+04-6.204956050D+02
    700.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26963.000
 0.000000000D+00 0.000000000D+00 1.714255083D+01 1.093131841D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.018779486D+05-6.764318260D+01
TiN(cr)            Chase,1998 pp1612-4.
 2 j 6/68 TI  1.00N   1.00    0.00    0.00    0.00 1   61.8737000    -337648.800
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5487.000
-5.479117220D+05 9.328691110D+03-6.386263890D+01 2.429925456D-01-4.304234520D-04
 3.792645100D-07-1.317412256D-10                -8.424256140D+04 3.392988560D+02
    800.000   3220.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5487.000
-3.656247060D+05 1.265730431D+03 3.831711190D+00 1.632900455D-03-1.062786626D-07
 1.310931390D-11-5.770548410D-16                -5.027654400D+04-1.652632899D+01
TiN(L)             Chase,1998 pp1612-4.
 1 j 6/68 TI  1.00N   1.00    0.00    0.00    0.00 2   61.8737000    -337648.800
   3220.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5487.000
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.626039860D+04-3.958296649D+01
TiO(a)             Alpha,monoclinic. Gurvich,1982 pt1 p98 pt2 p99.
 2 tpis82 TI  1.00O   1.00    0.00    0.00    0.00 1   63.8664000    -542000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6175.000
-1.126115023D+07 2.107240660D+05-1.601946203D+03 6.360717840D+00-1.380180278D-02
 1.563169158D-05-7.238514780D-09                -1.014208223D+06 8.368056830D+03
    500.000   1265.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6175.000
-2.066517895D+05 0.000000000D+00 8.243115270D+00-4.896702160D-03 3.806679150D-06
 0.000000000D+00 0.000000000D+00                -6.815384410D+04-4.265310470D+01
TiO(b)             Beta,cubic. Gurvich,1982 pt1 p98 pt2 p99.
 1 tpis82 TI  1.00O   1.00    0.00    0.00    0.00 2   63.8664000    -542000.000
   1265.000   1810.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6175.000
-1.400082506D+05 0.000000000D+00 6.173304260D+00 1.455287203D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.756357790D+04-3.249519859D+01
TiO(c)             Gamma,cubic. Gurvich,1982 pt1 p98 pt2 p99.
 1 tpis82 TI  1.00O   1.00    0.00    0.00    0.00 3   63.8664000    -542000.000
   1810.000   2030.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6175.000
 2.080459342D+05 0.000000000D+00 5.795530945D+00 1.404532558D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.627964090D+04-2.933709305D+01
TiO(L)             Liquid. Gurvich,1982 pt1 p98 pt2 p99.
 1 tpis82 TI  1.00O   1.00    0.00    0.00    0.00 4   63.8664000    -542000.000
   2030.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6175.000
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.314903830D+04-4.370051573D+01
TiO2(cr)           Rutile,tetragonal. Gurvich,1982 pt1 p105 pt2 p105.
 2 tpis82 TI  1.00O   2.00    0.00    0.00    0.00 1   79.8658000    -944000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.000
 1.712264157D+07-2.997059314D+05 2.143439285D+03-7.997230440D+00 1.661745261D-02
-1.817331921D-05 8.179403360D-09                1.253121023D+06-1.132509587D+04
    500.000   2185.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.000
-1.244201863D+05 0.000000000D+00 7.600577340D+00 1.421666301D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.162831515D+05-3.834053430D+01
TiO2(L)            Liquid. Gurvich,1982 pt1 p105 pt2 p105.
 1 tpis82 TI  1.00O   2.00    0.00    0.00    0.00 2   79.8658000    -944000.000
   2185.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8680.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.143261561D+05-6.551584491D+01
Ti2O3(I)           Hexagonal. Gurvich,1982 pt1 p109 pt2 p108.
 2 tpis82 TI  2.00O   3.00    0.00    0.00    0.00 1  143.7322000   -1520000.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14090.000
-1.771212920D+06 2.344459434D+04-1.110358342D+02 2.714352074D-01-1.921153675D-04
 0.000000000D+00 0.000000000D+00                -2.995932792D+05 6.382146810D+02
    400.000    464.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14090.000
 0.000000000D+00 0.000000000D+00 5.692590423D+01-2.558542837D-01 3.734811793D-04
 0.000000000D+00 0.000000000D+00                -1.917653868D+05-2.555304929D+02
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Ti2O3(I')          Hexagonal. Gurvich,1982 pt1 p109 pt2 p108.
 2 tpis82 TI  2.00O   3.00     0.00     0.00     0.00 2  143.7322000    -1520000.000
    464.000    580.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14090.000
 0.000000000D+00 0.000000000D+00 9.288208205D+01-2.728212486D-01 2.430399386D-04
 0.000000000D+00 0.000000000D+00                 -2.022790157D+05-4.543828632D+02
    580.000   2110.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14090.000
 4.228751905D+05 0.000000000D+00 1.281963700D+01 4.013104801D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.858705711D+05-6.399935229D+01
Ti2O3(L)           Liquid. Gurvich,1982 pt1 p109 pt2 p108.
 1 tpis82 TI  2.00O   3.00     0.00     0.00     0.00 3  143.7322000    -1520000.000
   2110.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          14090.000
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.821646342D+05-1.087120898D+02
Ti3O5(a)           Alpha,monoclinic. Gurvich,1982 pt1 p111 pt2 p110.
 2 tpis82 TI  3.00O   5.00     0.00     0.00     0.00 1  223.5980000    -2457000.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22630.000
 0.000000000D+00 0.000000000D+00 4.315304530D+00 4.637018750D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.988551027D+05-2.323385163D+01
    298.150    448.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22630.000
-2.175887695D+07 0.000000000D+00 1.012212506D+03-3.624156324D+00 3.726318087D-03
 0.000000000D+00 0.000000000D+00                 -5.421167010D+05-4.959468179D+03
Ti3O5(b)           Beta,rhombic. Gurvich,1982 pt1 p111 pt2 p110.
 1 tpis82 TI  3.00O   5.00     0.00     0.00     0.00 2  223.5980000    -2457000.000
    448.000   2050.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22630.000
 0.000000000D+00 0.000000000D+00 2.020131072D+01 5.124775844D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.004933224D+05-9.863577455D+01
Ti3O5(L)           Liquid. Gurvich,1982 pt1 p111 pt2 p110.
 1 tpis82 TI  3.00O   5.00     0.00     0.00     0.00 3  223.5980000    -2457000.000
   2050.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          22630.000
 0.000000000D+00 0.000000000D+00 3.127063411D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.923316313D+05-1.627424211D+02
Ti4O7(cr)          Triclinic. Gurvich,1982 pt1 p112 pt2 p111.
 2 tpis82 TI  4.00O   7.00     0.00     0.00     0.00 1  303.4638000    -3403000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          35630.000
 4.558528430D+06-8.146955640D+04 5.758643730D+02-1.933194123D+00 3.842536530D-03
-4.030781120D-06 1.748510017D-09                 -4.239230760D+04-3.066670887D+03
    500.000   1960.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          35630.000
-4.675287930D+05 0.000000000D+00 2.961388604D+01 5.773820220D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.199386150D+05-1.488468383D+02
Ti4O7(L)           Liquid. Gurvich,1982 pt1 p112 pt2 p111.
 1 tpis82 TI  4.00O   7.00     0.00     0.00     0.00 2  303.4638000    -3403000.000
   1960.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          35630.000
 0.000000000D+00 0.000000000D+00 4.353834441D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.142527640D+05-2.319810806D+02
U(a)               Alpha. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00     0.00     0.00     0.00 1  238.0289100          0.000
    200.000    942.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6364.000
-1.540899462D+04 2.318801962D+02 1.227944510D+00 7.136117480D-03-1.018038579D-05
 1.136884370D-08-3.669367430D-12                 -1.986921870D+03-2.035974193D+00
U(b)               Beta. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00     0.00     0.00     0.00 2  238.0289100          0.000
    942.000   1049.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6364.000
 0.000000000D+00 0.000000000D+00 5.099518793D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.672080149D+03-2.378030116D+01
U(c)               Gamma. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00     0.00     0.00     0.00 3  238.0289100          0.000
   1049.000   1408.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6364.000
 0.000000000D+00 0.000000000D+00 4.606404947D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.859187270D+02-1.980809042D+01
U(L)               Liquid. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00     0.00     0.00     0.00 4  238.0289100          0.000
   1408.000   4000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6364.000
-9.466562120D+04 8.526619680D+02 4.209128020D+00 8.407200810D-04-1.309545676D-07
 1.985020032D-11-1.231574075D-15                 -5.956398090D+03-1.667247672D+01
UF3(cr)            Hexagonal. Gurvich,1982 pt1 p209 pt2 p236.
 1 tpis82 U   1.00F   3.00     0.00     0.00     0.00 1  295.0241196    -1508700.000
    298.150   1768.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18380.000
-1.245413139D+05 0.000000000D+00 1.281362341D+01 8.479152710D-05 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.856957321D+05-5.889112439D+01
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UF3(L)              Liquid. Gurvich,1982 pt1 p209 pt2 p236.
 1 tpis82 U   1.00F   3.00     0.00     0.00     0.00 2  295.0241196   -1508700.000
   1768.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         18380.000
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.869060867D+05-8.091478353D+01
UF4(cr)             Monoclinic. Gurvich,1982 pt1 p212 pt2 p243.
 2 tpis82 U   1.00F   4.00     0.00     0.00     0.00 1  314.0225228   -1920500.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22550.000
-1.900846659D+06 3.555369140D+04-2.684351890D+02 1.162227739D+00-2.589319495D-03
 2.991673531D-06-1.405949560D-09                 -3.939232500D+05 1.401148993D+03
    500.000   1309.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22550.000
-1.687548936D+05 0.000000000D+00 1.670280525D+01-3.858715240D-03 3.366874970D-06
 0.000000000D+00 0.000000000D+00                 -2.363858828D+05-7.687256170D+01
UF4(L)              Liquid. Gurvich,1982 pt1 p212 pt2 p243.
 1 tpis82 U   1.00F   4.00     0.00     0.00     0.00 2  314.0225228   -1920500.000
   1309.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         22550.000
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.358206485D+05-9.894817389D+01
UF5(b)              Beta,tetragonal. Gurvich,1982 pt1 p217 pt2 p250.
 1 tpis82 U   1.00F   5.00     0.00     0.00     0.00 1  333.0209260   -2083000.000
    298.150    398.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26150.000
-2.315229641D+04 0.000000000D+00 1.505308190D+01 3.633166597D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.552530997D+05-6.539107895D+01
UF5(a)              Alpha,tetragonal. Gurvich,1982 pt1 p217 pt2 p250.
 1 tpis82 U   1.00F   5.00     0.00     0.00     0.00 2  333.0209260   -2083000.000
    398.000    621.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26150.000
-2.315229641D+04 0.000000000D+00 1.505308190D+01 3.633166597D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.542909264D+05-6.297355795D+01
UF5(L)              Liquid. Gurvich,1982 pt1 p217 pt2 p250.
 1 tpis82 U   1.00F   5.00     0.00     0.00     0.00 3  333.0209260   -2083000.000
    621.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         26150.000
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.524686368D+05-8.627305038D+01
UF6(cr)             Rhombic. Gurvich,1982 pt1 p222 pt2 p532.
 1 tpis82 U   1.00F   6.00     0.00     0.00     0.00 1  352.0193292   -2197700.000
    100.000    337.2107 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         31565.000
 1.490516238D+05-4.412150490D+03 5.041684430D+01-1.195638409D-01 2.070807828D-04
 0.000000000D+00 0.000000000D+00                 -2.502294955D+05-2.473731136D+02
UF6(L)              Liquid. Gurvich,1982 pt1 p222 pt2 p532.
 1 tpis82 U   1.00F   6.00     0.00     0.00     0.00 2  352.0193292   -2197700.000
    337.210   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         31565.000
 0.000000000D+00 0.000000000D+00 1.750554152D+01 1.611640373D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.680142931D+05-7.051080543D+01
UO2(cr)             Cubic. Gurvich,1982 pt1 p190 pt2 p209.
 2 tpis82 U   1.00O   2.00     0.00     0.00     0.00 1  270.0277100   -1085000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11280.000
-1.712140039D+07 3.206174610D+05-2.435851508D+03 9.665099460D+00-2.095506138D-02
 2.371859464D-05-1.097936236D-08                 -1.574556829D+06 1.272869884D+04
    500.000   3123.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11280.000
-2.775509993D+05 0.000000000D+00 1.161094006D+01-3.430918270D-03 2.044412020D-06
 0.000000000D+00 0.000000000D+00                 -1.347529024D+05-5.751912860D+01
UO2(L)              Liquid. Gurvich,1982 pt1 p190 pt2 p209.
 1 tpis82 U   1.00O   2.00     0.00     0.00     0.00 2  270.0277100   -1085000.000
   3123.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         11280.000
 0.000000000D+00 0.000000000D+00 1.575558872D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.342007409D+05-8.859616713D+01
UO2F2(cr)           Hexagonal. Gurvich,1982 pt1 p227 pt2 p262.
 2 tpis82 U   1.00O   2.00F    2.00     0.00     0.00 1  308.0245164   -1653600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19700.000
 2.774535231D+06-5.047416500D+04 3.733097480D+02-1.349660046D+00 2.816624451D-03
-3.086048235D-06 1.391361959D-09                 2.724906305D+04-1.962630228D+03
    500.000   2100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         19700.000
-1.227714401D+05 0.000000000D+00 1.277741930D+01 3.406816370D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -2.032540376D+05-5.821006900D+01
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UO3(c)              Gamma,monoclinic. Gurvich,1982 pt1 p195 pt2 p217.
 2 tpis82 U   1.00O   3.00    0.00    0.00    0.00 1  286.0271100   -1223800.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14585.000
-1.956676511D+06 3.951756640D+04-3.223198540D+02 1.417862899D+00-3.236211090D-03
 3.806716410D-06-1.814492554D-09                 -3.239008630D+05 1.660601808D+03
    500.000   3000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         14585.000
-2.090516805D+05 0.000000000D+00 1.271766576D+01-2.508681376D-03 2.295592116D-06
 0.000000000D+00 0.000000000D+00                 -1.515901509D+05-6.143076620D+01
U3O8(II)            Rhombic. Gurvich,1982 pt1 p199 pt2 p222.
 2 tpis82 U   3.00O   8.00    0.00    0.00    0.00 1  842.0819300   -3574800.000
    200.000    300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         42740.000
-1.312654971D+05 0.000000000D+00 1.981648464D+01 3.463180280D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -4.378350230D+05-8.998750380D+01
    300.000    483.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         42740.000
-2.819324251D+06 0.000000000D+00 1.227600892D+02-2.415563843D-01 0.000000000D+00
 3.622285580D-07 0.000000000D+00                 -4.659833440D+05-6.124926920D+02
U3O8(I)             Hexagonal. Gurvich,1982 pt1 p199 pt2 p222.
 1 tpis82 U   3.00O   8.00    0.00    0.00    0.00 2  842.0819300   -3574800.000
    483.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         42740.000
-5.848811295D+04 0.000000000D+00 2.988522475D+01 6.597141623D-03-4.626851131D-07
 0.000000000D+00 0.000000000D+00                 -4.394086740D+05-1.388063306D+02
U4O9(III)           Cubic. Gurvich,1982 pt1 p201 pt2 p223.
 1 tpis82 U   4.00O   9.00    0.00    0.00    0.00 1 1096.1102400   -4512000.000
    298.150    348.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         50750.000
-1.274607283D+08 0.000000000D+00 6.797154853D+03-2.205931654D+01 0.000000000D+00
 4.712462238D-05 0.000000000D+00                 -2.109373967D+06-3.324352924D+04
U4O9(II)            Cubic. Gurvich,1982 pt1 p201 pt2 p223.
 2 tpis82 U   4.00O   9.00    0.00    0.00    0.00 2 1096.1102400   -4512000.000
    348.000    380.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         50750.000
 6.572378889D+07 0.000000000D+00-1.352246013D+03 2.459469770D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.013155679D+04 7.375484389D+03
    380.000   1398.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         50750.000
-7.968840016D+05 0.000000000D+00 4.574063896D+01-1.083792070D-02 9.691491140D-06
 0.000000000D+00 0.000000000D+00                 -5.582419360D+05-2.211132773D+02
U4O9(I)             Gurvich,1982 pt1 p201 pt2 p223.
 1 tpis82 U   4.00O   9.00    0.00    0.00    0.00 3 1096.1102400   -4512000.000
   1398.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         50750.000
-3.094590060D+05 0.000000000D+00 3.592971805D+01 1.009247689D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.555228520D+05-1.695188988D+02
V(cr)               Crystal. Ref-Elm. Chase,1998 p1917.
 3 j 6/73 V   1.00    0.00    0.00    0.00    0.00 1   50.9415000          0.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4640.000
 2.845125913D+05-5.094932860D+03 3.715018720D+01-1.176030941D-01 2.255823526D-04
-2.260642686D-07 9.289596800D-11                 2.254378204D+04-1.968241679D+02
    600.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4640.000
 1.372056465D+06-7.847553620D+03 2.095142247D+01-2.055640932D-02 1.323266530D-05
-4.042182900D-09 5.087521100D-13                 4.374800000D+04-1.292763446D+02
   1400.000   2190.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4640.000
 5.281067680D+08-1.907420191D+06 2.862656637D+03-2.277492896D+00 1.017078880D-03
-2.412149691D-07 2.377114537D-11                 1.169890783D+07-1.956716732D+04
V(L)                Liquid. Ref-Elm. Chase,1998 p1917.
 1 j 6/73 V   1.00    0.00    0.00    0.00    0.00 2   50.9415000          0.000
   2190.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4640.000
 0.000000000D+00 0.000000000D+00 5.557032224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.899700630D+03-3.070532450D+01
VCL2(cr)            Pankratz,1984.
 1 g10/00 V   1.00CL  2.00    0.00    0.00    0.00 1  121.8475000    -451872.000
    298.000   1300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
-3.844575327D+04 0.000000000D+00 8.648281619D+00 1.435173931D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -5.711862150D+04-3.824393774D+01
VCL3(cr)            Pankratz,1984.
 1 g 8/00 V   1.00CL  3.00    0.00    0.00    0.00 1  157.3005000    -581115.760
    298.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
-1.163436931D+05 0.000000000D+00 1.218941730D+01 1.091980165D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -7.396479110D+04-5.467967609D+01
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VN(cr)              Chase,1998 p1635.
 2 j12/73 V   1.00N   1.00    0.00    0.00    0.00 1   64.9482000    -217150.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6225.792
 2.091900078D+05-3.051142421D+03 1.689002455D+01-2.016563261D-02 2.024805796D-05
-9.052281300D-09 1.375923345D-12                -1.233229950D+04-9.561817060D+01
   1000.000   3500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6225.792
 8.212748990D+05-2.203406736D+03 6.907596040D+00 1.164274622D-03-3.307430080D-07
 1.061954757D-10-1.105176783D-14                -1.341131421D+04-3.925480780D+01
VO(cr)              Cubic Gurvich,1982 pt1 p60 pt2 p63.
 2 tpis82 V   1.00O   1.00    0.00    0.00    0.00 1   66.9409000    -430800.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5980.000
-2.040260824D+07 3.783102280D+05-2.848005957D+03 1.118080448D+01-2.407270159D-02
 2.710471323D-05-1.249526447D-08                -1.758506851D+06 1.490654242D+04
    500.000   2063.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5980.000
-1.970015037D+05 0.000000000D+00 6.365723760D+00 1.576630310D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.444168120D+04-3.381741570D+01
VO(L)               Liquid Gurvich,1982 pt1 p60 pt2 p63.
 1 tpis82 V   1.00O   1.00    0.00    0.00    0.00 2   66.9409000    -430800.000
   2063.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5980.000
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.921350390D+04-4.329727468D+01
V2O3(cr)            Hexagonal. Gurvich,1982 pt1 p65 pt2 p67.
 2 tpis82 V   2.00O   3.00    0.00    0.00    0.00 1  149.8812000   -1216800.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17130.000
-2.445935804D+07 4.555627240D+05-3.448966200D+03 1.365879117D+01-2.955666350D-02
 3.340613030D-05-1.544661718D-08                -2.200372063D+06 1.802928653D+04
    500.000   2230.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17130.000
-4.148342860D+05 0.000000000D+00 1.735995875D+01-2.248234102D-03 1.310940149D-06
 0.000000000D+00 0.000000000D+00                -1.528252156D+05-8.926688900D+01
V2O3(L)             Liquid. Gurvich,1982 pt1 p65 pt2 p67.
 1 tpis82 V   2.00O   3.00    0.00    0.00    0.00 2  149.8812000   -1216800.000
   2230.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         17130.000
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.407455834D+05-9.794985841D+01
V2O4(II)            Monoclinic. Gurvich,1982 pt1 p67 pt2 p68.
 1 tpis82 V   2.00O   4.00    0.00    0.00    0.00 1  165.8806000   -1432600.000
    200.000    338.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16720.000
-4.872822280D+05 0.000000000D+00 4.755837160D+01-1.909710602D-01 3.188918050D-04
 0.000000000D+00 0.000000000D+00                -1.824442970D+05-2.197380006D+02
V2O4(I)             Tetragonal. Gurvich,1982 pt1 p67 pt2 p68.
 1 tpis82 V   2.00O   4.00    0.00    0.00    0.00 2  165.8806000   -1432600.000
    338.700   1818.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16720.000
-3.456246971D+05 0.000000000D+00 1.740258897D+01 2.292498295D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.776670154D+05-8.737764367D+01
V2O4(L)             Liquid. Gurvich,1982 pt1 p67 pt2 p68.
 1 tpis82 V   2.00O   4.00    0.00    0.00    0.00 3  165.8806000   -1432600.000
   1818.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         16720.000
 0.000000000D+00 0.000000000D+00 2.164890054D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.679377747D+05-1.076187785D+02
V2O5(cr)            Rhombic. Gurvich,1982 pt1 p68 pt2 p69.
 2 tpis82 V   2.00O   5.00    0.00    0.00    0.00 1  181.8800000   -1551000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21210.000
-1.149585895D+07 2.200852292D+05-1.711429444D+03 6.997610220D+00-1.543892990D-02
 1.771425949D-05-8.283987620D-09                -1.174509299D+06 8.899979010D+03
    500.000    954.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21210.000
-4.708328420D+05 0.000000000D+00 2.297387367D+01-1.118831481D-02 1.146815480D-05
 0.000000000D+00 0.000000000D+00                -1.945738450D+05-1.150219507D+02
V2O5(L)             Liquid. Gurvich,1982 pt1 p68 pt2 p69.
 1 tpis82 V   2.00O   5.00    0.00    0.00    0.00 2  181.8800000   -1551000.000
    954.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21210.000
 0.000000000D+00 0.000000000D+00 2.285161723D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.880385445D+05-1.113109611D+02
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W(cr)              Crystal. Ref-Elm. Chase,1998 pp1925-8.
 4 j 6/66 W   1.00    0.00    0.00    0.00    0.00 1  183.8400000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4973.000
-6.824541400D+03-2.254249090D+02 4.976604610D+00-6.926436340D-03 1.202272986D-05
-9.344133510D-09 2.818887123D-12                -3.510679270D+00-2.361334984D+01
   1000.000   2600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4973.000
 5.530134840D+05-2.041485344D+03 5.870839470D+00-1.920714198D-03 1.067652983D-06
-2.355109022D-10 2.160679310D-14                 1.163812518D+04-3.319171800D+01
   2600.000   3200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4973.000
 2.474736879D+09 4.488921620D+06-1.235978300D+04 9.678565660D+00-3.556364610D-03
 6.380420610D-07-4.521123450D-11                -2.029500909D+07 8.274369690D+04
   3200.000   3680.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4973.000
-1.755550399D+10 1.179059156D+07 1.177715365D+03-2.675166841D+00 7.252172480D-04
-6.128007580D-08 0.000000000D+00                -9.702249190D+07-1.148926234D+03
W(L)               Liquid. Ref-Elm. Chase,1998 pp1925-8.
 1 j 6/66 W   1.00    0.00    0.00    0.00    0.00 2  183.8400000          0.000
   3680.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4973.000
 0.000000000D+00 0.000000000D+00 4.277341659D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.755443078D+03-2.086449853D+01
WC(cr)             Hf:Wagman,1982 p203. Barin,1989 pt2 p1642.
 1 bar 89 W   1.00C   1.00    0.00    0.00    0.00 1  195.8507000      -40540.000
    298.150   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-1.119754391D+05-5.553268210D-01 5.217965240D+00 1.037888263D-03-1.229060652D-07
 2.880427321D-13-7.236307119D-17                -6.848998700D+03-2.677066218D+01
WCL6(I)            Alpha1. Chase,1998 pp931-4.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 1  396.5580000     -593710.000
    298.150    450.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 1.661826519D+02 0.000000000D+00 1.508873100D+01 2.015651227D-02-2.754798370D-08
 0.000000000D+00 0.000000000D+00                -7.680028810D+04-6.329365920D+01
WCL6(II)           Alpha2. Chase,1998 pp931-4.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 2  396.5580000     -593710.000
    450.000    503.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-9.897046360D+03 0.000000000D+00 1.522857952D+01 1.994376611D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.636166220D+04-6.296167010D+01
WCL6(III)          Beta. Chase,1998 pp931-4.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 3  396.5580000     -593710.000
    503.000    555.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 2.264474996D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.565217840D+04-9.527165358D+01
WCL6(L)            Liquid. Chase,1998 pp931-4.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 4  396.5580000     -593710.000
    555.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 2.415439996D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.568493560D+04-1.033604557D+02
WOCL4(cr)          Crystal. Chase,1998 pp897-9.
 1 j 3/67 W   1.00O   1.00CL  4.00    0.00    0.00 1  341.6514000     -671114.000
    298.150    484.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 1.295153216D+03 0.000000000D+00 1.378522135D+01 1.276179773D-02-1.713279395D-07
 0.000000000D+00 0.000000000D+00                -8.538742740D+04-6.154983780D+01
WOCL4(L)           Liquid. Chase,1998 pp897-9.
 1 j 3/67 W   1.00O   1.00CL  4.00    0.00    0.00 2  341.6514000     -671114.000
    484.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 0.000000000D+00 0.000000000D+00 2.188992496D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.236656270D+04-9.422321377D+01
WO2(cr)            Gurvich,1982 pt1 p46 pt2 p49.
 2 tpis82 W   1.00O   2.00    0.00    0.00    0.00 1  215.8388000     -588100.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             8711.000
-1.733842408D+04 0.000000000D+00 2.558979845D+00 1.457260175D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.220058630D+04-1.293182268D+01
    298.150   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             8711.000
-1.555714047D+05 0.000000000D+00 7.983272616D+00 1.595163155D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.370467050D+04-4.074555290D+01
WO2CL2(cr)         Chase,1998 p848.
 1 j 3/67 W   1.00O   2.00CL  2.00    0.00    0.00 1  286.7448000     -780316.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-3.819410020D+05 2.367029691D+03 9.834455770D+00-2.508443012D-02 1.017169638D-04
-1.040117941D-07 3.468311980D-11                -1.111440350D+05-2.227929881D+01
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WO3(III)          Gurvich,1982 pt1 p49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 1  231.8382000    -841300.000
    100.000    325.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13280.000
-2.841140443D+05 7.257714840D+03-6.708405120D+01 3.092936300D-01-4.127635650D-04
 0.000000000D+00 0.000000000D+00                -1.335884160D+05 3.409113710D+02
WO3(III,II)       Gurvich,1982 pt1 p49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 2  231.8382000    -841300.000
    325.000   1013.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13280.000
-5.186114395D+04 0.000000000D+00 8.548308920D+00 4.317151582D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.040935177D+05-4.044670662D+01
WO3(I)            Gurvich,1982 pt1 p49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 3  231.8382000    -841300.000
   1013.000   1747.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13280.000
 0.000000000D+00 0.000000000D+00 9.737555190D+00 1.958624140D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.039166330D+05-4.614390358D+01
WO3(L)            Liquid. Gurvich,1982 pt1 p49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 4  231.8382000    -841300.000
   1747.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13280.000
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.022412072D+05-8.082927535D+01
Zn(cr)            Crystal. Ref-Elm. Cox,1989 p221.
 1 coda89 ZN  1.00    0.00    0.00    0.00    0.00 1   65.3900000          0.000
    200.000    692.7307 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5657.000
 3.702080380D+05-5.915475500D+03 3.959500360D+01-1.143735885D-01 1.934363797D-04
-1.675385126D-07 6.078189940D-11                2.681737238D+04-2.114848186D+02
Zn(L)             Liquid. Ref-Elm. Cox,1989 p221.
 1 coda89 ZN  1.00    0.00    0.00    0.00    0.00 2   65.3900000          0.000
    692.730   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5657.000
 0.000000000D+00 0.000000000D+00 3.776530427D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.317345880D+02-1.567077937D+01
ZnSO4(a)          Alpha. Chase,1998 p1788.
 1 j 3/79 ZN  1.00S   1.00O   4.00    0.00    0.00 1  161.4526000    -980143.840
    200.000    540.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17238.080
 4.103530390D+05-7.357987120D+03 5.215317850D+01-1.152180317D-01 1.922132213D-04
-1.099361720D-07 0.000000000D+00                -8.649370210D+04-2.794432413D+02
ZnSO4(a')         Alpha'.Chase,1998 p1788.
 1 j 3/79 ZN  1.00S   1.00O   4.00    0.00    0.00 2  161.4526000    -980143.840
    540.000   1013.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17238.080
-3.253792010D+06 3.252313710D+04-1.146490609D+02 2.718567520D-01-3.079986965D-04
 1.830520033D-07-4.445112450D-11                -2.895173465D+05 6.881710230D+02
ZnSO4(b)          Beta. Chase,1998 p1788.
 1 j 3/79 ZN  1.00S   1.00O   4.00    0.00    0.00 3  161.4526000    -980143.840
   1013.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17238.080
 0.000000000D+00 0.000000000D+00 1.746161830D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.211366813D+05-8.514209609D+01
Zr(a)             Alpha. Ref-Elm. Chase,1998 pp1943-7.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 1   91.2240000          0.000
    200.000   1135.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5497.000
-1.153699220D+04 2.626203401D+01 2.932054698D+00 5.743358570D-04-7.651710410D-07
 1.597202829D-09-6.097129620D-13                -1.084153260D+03-1.215776960D+01
Zr(b)             Beta. Ref-Elm. Chase,1998 pp1943-7.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 2   91.2240000          0.000
   1135.000   2125.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5497.000
-1.065463955D+06 4.273000010D+03-3.173856480D+00 5.018842560D-03-2.363431747D-06
 7.707582390D-10-8.156156570D-14                -2.641247444D+04 3.072041827D+01
Zr(L)             Liquid. Ref-Elm. Chase,1998 pp1943-7.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 3   91.2240000          0.000
   2125.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5497.000
 0.000000000D+00 0.000000000D+00 5.032166658D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.100795852D+03-2.548066000D+01
ZrC(cr)           Crystal. Chase,1998 pp658-60.
 2 j12/64 ZR  1.00C   1.00    0.00    0.00    0.00 1  103.2347000    -196648.000
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5862.000
-1.329596558D+05 1.766908163D+03-9.907099000D+00 5.427909170D-02-8.887722520D-05
 7.332246190D-08-2.420411623D-11                -3.297124410D+04 5.279964170D+01
    800.000   3805.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5862.000
 8.297591180D+05-4.224196050D+03 1.308509211D+01-5.018095870D-03 2.155019459D-06
-4.233046770D-10 3.266859200D-14                -7.112782350D+02-7.921945570D+01
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ZrC(L)              Liquid. Chase,1998 pp658-60.
 1 j12/64 ZR  1.00C   1.00     0.00     0.00     0.00 2  103.2347000     -196648.000
   3805.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           5862.000
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.885005134D+04-3.953387107D+01
ZrN(cr)             Chase,1998 pp1617-9 6/61.
 2 g11/00 ZR  1.00N   1.00     0.00     0.00     0.00 1  105.2307000     -371238.000
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6590.000
 2.548624207D+05-4.476456170D+03 2.958601499D+01-6.635810940D-02 1.033814686D-04
-8.272994600D-08 2.689947231D-11                 -2.492379728D+04-1.616084405D+02
    800.000   3225.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6590.000
 2.174089790D+05-1.074470994D+03 7.053124150D+00-1.447713245D-04 3.458043010D-07
-5.893486000D-11 3.787112980D-15                 -3.999164210D+04-3.811591880D+01
ZrN(L)              Chase,1998 pp1617-9 6/61.
 1 g11/00 ZR  1.00N   1.00     0.00     0.00     0.00 2  105.2307000     -371238.000
   3225.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           6590.000
 0.000000000D+00 0.000000000D+00 7.045033321D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -3.882762780D+04-3.444078302D+01
ZrO2(III)           Monoclinic. Gurvich,1982 pt1 p123 pt2 p122.
 2 tpis82 ZR  1.00O   2.00     0.00     0.00     0.00 1  123.2228000    -1100300.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8751.000
-4.214621830D+06 7.918732350D+04-6.071267910D+02 2.463358622D+00-5.388665930D-03
 6.144154000D-06-2.860860736D-09                 -4.893051030D+05 3.163542730D+03
    500.000   1445.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8751.000
-1.616911113D+05 0.000000000D+00 8.218464380D+00 1.091902502D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.353760676D+05-4.200007680D+01
ZrO2(II)            Tetragonal. Gurvich,1982 pt1 p123 pt2 p122.
 1 tpis82 ZR  1.00O   2.00     0.00     0.00     0.00 2  123.2228000    -1100300.000
   1445.000   2620.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8751.000
 0.000000000D+00 0.000000000D+00 9.393217399D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.348114469D+05-4.823174581D+01
ZrO2(I)             Cubic. Gurvich,1982 pt1 p123 pt2 p122.
 1 tpis82 ZR  1.00O   2.00     0.00     0.00     0.00 3  123.2228000    -1100300.000
   2620.000   2983.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8751.000
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.338466275D+05-4.943361269D+01
ZrO2(L)             Liquid. Gurvich,1982 pt1 p123 pt2 p122.
 1 tpis82 ZR  1.00O   2.00     0.00     0.00     0.00 4  123.2228000    -1100300.000
   2983.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8751.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 -1.301975851D+05-6.505001424D+01
END PRODUCTS
Air                 Mole%:N2 78.084,O2 20.9476,Ar .9365,CO2 .0319.Gordon,1982.Reac
 2 g 9/95 N 1.5617O .41959AR.00937C .00032  .00000 0   28.9651159      -125.530
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8649.264
 1.009950160D+04-1.968275610D+02 5.009155110D+00-5.761013730D-03 1.066859930D-05
-7.940297970D-09 2.185231910D-12                 -1.767967310D+02-3.921504225D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           8649.264
 2.415214430D+05-1.257874600D+03 5.144558670D+00-2.138541790D-04 7.065227840D-08
-1.071483490D-11 6.577800150D-16                  6.462263190D+03-8.147411905D+00
B2H6(L)             Diborane. McBride,1996 pp84,92.
 0 g 6/96 B   2.00H   6.00     0.00     0.00     0.00 1   27.6696400      16445.000
    180.590      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
B5H9(L)             Pentaborane. Chase,1998 p302.
 0 j 3/65 B   5.00H   9.00     0.00     0.00     0.00 1   63.1264600      42840.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
(CH2)x(cr)          Ethylene polymer. McBride,1996 pp84,92.
 0 g 6/96 C   1.00H   2.00     0.00     0.00     0.00 1   14.0265800     -25600.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
CH3NO2(L)           Nitromethane. McBride,1996 pp85,93.
 0 g 6/96 C   1.00H   3.00N   1.00O   2.00     0.00 1   61.0400200     -113100.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
CH4(L)              Methane. McBride,1996 pp85,93.
 0 g 6/96 C   1.00H   4.00     0.00     0.00     0.00 1   16.0424600      -89233.000
    111.643      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
CH3OH(L)            MeOH. TRC(12/87) p5000 (12/84)tc,uc,vc5031,5033.       React.
 1 n12/84 C   1.00H   4.00O   1.00     0.00     0.00 1   32.0418600     -238910.000
    175.610    390.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18995.000
-1.302004763D+06 3.166984180D+04-3.031242152D+02 1.602231130D+00-4.594507340D-03
 6.990178310D-06-4.207388950D-09                 -1.656168201D+05 1.514346642D+03
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CH6N2(L)            Monomethyl Hydrazine. TRC(12/93) p9220.
 0 n12/93 C   1.00H   6.00N   2.00     0.00     0.00 1   46.0717400      54200.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C2H2(L),acetyle     Acetylene. McBride,1996 pp84,92.
 0 g 6/96 C   2.00H   2.00     0.00     0.00     0.00 1   26.0372800     207599.000
    192.350      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
CH3CN(L)            Ethanenitrile (Acetonitrile). McBride,1996 pp84,92.
 0 g 6/96 C   2.00H   3.00N   1.00     0.00     0.00 1   41.0519200      31380.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C2H4(L)             Ethylene. McBride,1996 pp84,92.
 0 g 6/96 C   2.00H   4.00     0.00     0.00     0.00 1   28.0531600      33945.000
    169.420      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C2H4O(L),ethyle     Ethylene oxide (Oxirane). McBride,1996 pp84,92.
 0 g 6/96 C   2.00H   4.00O   1.00     0.00     0.00 1   44.0525600     -78841.000
    283.650      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C2H6(L)             Ethane. McBride,1996 pp84,92.
 0 g 6/96 C   2.00H   6.00     0.00     0.00     0.00 1   30.0690400    -103819.000
    184.559      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C2H5OH(L)           Ethanol. TRC(12/87) p5000 (12/84) tc,uc,vc5031-3.        React.
 1 n12/84 C   2.00H   6.00O   1.00     0.00     0.00 1   46.0684400    -277510.000
    159.000    390.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            24082.000
 4.501115940D+05-1.020828990D+04 1.014266780D+02-3.874672610D-01 7.121392610D-04
-1.857071450D-07-2.037622570D-10                 7.448557900D+03-5.044255520D+02
C2H8N2(L),UDMH      Unsymmetrical Dimethyl Hydrazine. McBride,1996 pp85,93.
 0 g 6/96 C   2.00H   8.00N   2.00     0.00     0.00 1   60.0983200      48900.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C2N2(L)             Cyanogen. McBride,1996 pp84,92.
 0 g 6/96 C   2.00N   2.00     0.00     0.00     0.00 1   52.0348000     283209.000
    252.050      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C3H6(L),propyle     Propylene. McBride,1996 pp85,93.
 0 g 6/96 C   3.00H   6.00     0.00     0.00     0.00 1   42.0797400      -2704.000
    225.460      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C3H7NO3(L)          Propyl Nitrate. McBride,1996 pp85,93.
 0 g 6/96 C   3.00H   7.00N   1.00O    3.00     0.00 1  105.0925800    -214500.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C3H8(L)             Propane. McBride,1996 pp85,93.
 0 g 6/96 C   3.00H   8.00     0.00     0.00     0.00 1   44.0956200    -128228.000
    231.076      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C4H8(L),1-buten     1-Butene. McBride,1996 pp84,92.
 0 g 6/96 C   4.00H   8.00     0.00     0.00     0.00 1   56.1063200     -25173.000
    266.920      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C4H10(L),n-buta     n-Butane. McBride,1996 pp84,92.
 0 g 6/96 C   4.00H  10.00     0.00     0.00     0.00 1   58.1222000    -150664.000
    272.638      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C4H10(L),isobut     Isobutane(2-methyl propane). McBride,1996 pp84,92.
 0 g 6/96 C   4.00H  10.00     0.00     0.00     0.00 1   58.1222000    -159664.000
    261.361      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C5H12(L),n-pent     n-Pentane. McBride,1996 pp85,93.
 0 g 6/96 C   5.00H  12.00     0.00     0.00     0.00 1   72.1487800    -173490.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0             0.000
C6H6(L)             TRC(10/86) tc,uc,vc3201 (4/83) p3200.                    React.
 1 n10/86 C   6.00H   6.00     0.00     0.00     0.00 1   78.1118400      49080.000
    278.680    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            30110.000
-2.291003940D+06 3.692058160D+04-1.820019971D+02 2.634137216D-01 9.742585920D-04
-3.307909150D-06 2.888191394D-09                -1.730169095D+05 1.070458659D+03
C6H5NH2(L)          Aniline. TRC(12/88) tc,uc,vc9370. TRC(6/95) p9370.       React.
 1 n12/88 C   6.00H   7.00N   1.00     0.00     0.00 1   93.1264800      31500.000
    267.130    460.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            34020.000
 6.257653490D+07-8.930118090D+05 5.055201440D+03-1.397470822D+01 1.889729680D-02
-9.205910240D-06-1.289458554D-09                 4.267459270D+06-2.801220752D+04
C6H14(L),n-hexa     n-hexane. TRC(4/85) p,tc,uc,vc1440,1441.                 React.
 1 n 4/85 C   6.00H  14.00     0.00     0.00     0.00 1   86.1753600    -198660.000
    177.860    300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            46920.000
 7.721016130D+06-2.249298616D+05 2.717090647D+03-1.698251992D+01 5.907215180D-02
-1.074528475D-04 8.024238270D-08                 8.808691730D+05-1.292771483D+04
C7H8(L)             TRC(10/86) tc uc vc3200-1 (4/83) p-3200.                 React.
 1 n10/86 C   7.00H   8.00     0.00     0.00     0.00 1   92.1384200      12180.000
    178.150    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            33470.000
-3.713549510D+06 7.772529030D+04-6.312269860D+02 2.724391982D+00-6.103535080D-03
 7.022421900D-06-3.113715680D-09                -3.452115500D+05 3.265980710D+03
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C7H16(L),n-hept   TRC(10/84) p-1010 (10/75) tc,uc,vc1460.                    React.
 1 n10/75 C   7.00H  16.00    0.00    0.00    0.00 1  100.2019400    -224350.000
    182.580    380.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        52640.000
 1.759947367D+06-3.749396790D+04 3.963064900D+02-2.117827431D+00 6.828248670D-03
-1.131862116D-05 7.736860130D-09                 1.269072572D+05-1.921686840D+03
C8H18(L),n-octa   TRC(10/76) tc,uc,vc1491,1492. Hf:(10/84) p1010.           React.
 1 n10/84 C   8.00H  18.00    0.00    0.00    0.00 1  114.2285200    -250260.000
    216.370    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        61490.000
-1.683314826D+07 3.532615080D+05-2.967857531D+03 1.316703807D+01-3.186822410D-02
 4.075748010D-05-2.153277285D-08                -1.588494258D+06 1.521639569D+04
C8H18(L),isooct   TRC(10/76) tc,uc,vc1491,1492. Hf:(10/82) p1490.           React.
 1 n10/82 C   8.00H  18.00    0.00    0.00    0.00 1  114.2285200    -259160.000
    165.790    380.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        50190.000
 1.419157943D+05-2.937251288D+03 4.168834760D+01-8.436942210D-02 2.894147919D-04
-2.200563712D-07 7.234225570D-11                -2.479398829D+04-1.930220201D+02
CLF3(L)           Chlorine Trifluoride. McBride,1996 pp84,92.
 0 g 6/96 CL  1.00F   3.00    0.00    0.00    0.00 1   92.4482096    -193386.000
    284.890      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
CLO3F             Hf:Wagman,1982 p49. Chase,1998 p755.                       React.
 2 g 5/95 CL  1.00O   3.00F   1.00    0.00    0.00 0  102.4496032     -23800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13298.823
 4.461077310D+04-5.892352210D+02 3.558850810D+00 2.809585831D-02-3.610880350D-05
 2.273331859D-08-5.716733040D-12                -1.388667752D+03 4.590741392D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13298.823
-3.910495440D+05-1.193220687D+03 1.388657545D+01-3.541312060D-04 7.825464770D-08
-8.978325430D-12 4.163869660D-16                -1.275082535D+03-5.106452991D+01
CLO3F(L)          Perchloryl Fluoride. McBride,1996 pp85,93.
 0 g 6/96 CL  1.00O   3.00F   1.00    0.00    0.00 1  102.4496032     -47436.000
    226.400      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
CL2(L)            Chlorine. McBride,1996 pp84,92.
 0 g 6/96 CL  2.00    0.00    0.00    0.00    0.00 1   70.9060000     -22550.000
    239.120      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
F2(L)             Fluorine. McBride,1996 pp84,92.
 0 g 6/96 F   2.00    0.00    0.00    0.00    0.00 1   37.9968064     -13091.000
     85.020      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
F2O(L)            Oxygen Difluoride. McBride,1996 pp85,93.
 0 g 6/96 F   2.00O   1.00    0.00    0.00    0.00 1   53.9962064       6672.000
    128.400      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
HNO3(L)           Nitric Acid. McBride,1996 pp85,93.
 0 g 6/96 H   1.00N   1.00O   3.00    0.00    0.00 1   63.0128400    -173013.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
H2(L)             Hydrogen. McBride,1996 pp84,92.
 0 g 6/96 H   2.00    0.00    0.00    0.00    0.00 1    2.0158800       -9012.000
     20.270      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
H2O2(L)           Gurvich, 1989 v1 pt1 p126 pt2 p303.                        React.
 1 tpis89 H   2.00O   2.00    0.00    0.00    0.00 1   34.0146800    -187780.000
    272.740   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22949.000
 0.000000000D+00 0.000000000D+00 1.074386825D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.578789845D+04-4.803221291D+01
IRFNA             Inhibited Red Fuming Nitric Acid. McBride,1996 pp84,93.
 0 g 6/96 H   1.57N   1.63O   4.70F   0.02    0.00 1   99.9905349    -270496.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
JP-4              McBride,1996 pp85,93. Hcomb = 18640.BTU/#
 0 g 6/96 C   1.00H   1.94    0.00    0.00    0.00 1   13.9661036     -22723.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
JP-5              Or ASTMA1(L). McBride,1996 pp85,93. Hcomb = 18600.BTU/#
 0 g 6/96 C   1.00H   1.92    0.00    0.00    0.00 1   13.9459448     -22183.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
JP-10(L)          Exo-tetrahydrodicyclopentadiene. Smith,1979.                React.
 0 g 6/01 C  10.00H  16.00    0.00    0.00    0.00 0  136.2340400    -122800.400
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
JP-10(g)          Exo-tetrahydrodicyclopentadiene.Pri.Com.R.Jaffe 12/00.  React.
 2 g 6/01 C  10.00H  16.00    0.00    0.00    0.00 0  136.2340400     -86855.900
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22997.434
-7.310769440D+05 1.521764245D+04-1.139312644D+02 4.281501620D-01-5.218740440D-04
 3.357233400D-07-8.805750980D-11                -8.067482120D+04 6.320148610D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22997.434
 1.220329594D+07-5.794846240D+04 1.092281156D+02-1.082406215D-02 2.034992622D-06
-2.052060369D-10 8.575760210D-15                3.257334050D+05-7.092350760D+02
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Jet-A(L)          McBride,1996. Faith,1971. Gracia-Salcedo,1988.          React.
 1 g 2/96 C  12.00H  23.00    0.00    0.00    0.00 1  167.3110200    -303403.000
    220.000    550.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
-4.218262130D+05-5.576600450D+03 1.522120958D+02-8.610197550D-01 3.071662234D-03
-4.702789540D-06 2.743019833D-09                -3.238369150D+04-6.781094910D+02
Jet-A(g)          McBride,1996. Faith,1971. Gracia-Salcedo,1988.          React.
 2 g 8/01 C  12.00H  23.00    0.00    0.00    0.00 0  167.3110200    -249657.000
    273.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
-6.068695590D+05 8.328259590D+03-4.312321270D+01 2.572390455D-01-2.629316040D-04
 1.644988940D-07-4.645335140D-11                -7.606962760D+04 2.794305937D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 1.858356102D+07-7.677219890D+04 1.419826133D+02-7.437524530D-03 5.856202550D-07
 1.223955647D-11-3.149201922D-15                4.221989520D+05-8.986061040D+02
LiCLO4(cr)        Lithium Perchlorate. Chase,1998 p782.
 0 g 6/96 LI  1.00CL  1.00O   4.00    0.00    0.00 1  106.3916000    -380700.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
NF3(L)            Nitrogen trifluoride. McBride,1996 pp85,93.
 0 g 6/96 N   1.00F   3.00    0.00    0.00    0.00 1   71.0019096    -150387.000
    144.090      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
NH3(L)            Ammonia. McBride,1996 pp84,92.
 0 g 6/96 N   1.00H   3.00    0.00    0.00    0.00 1   17.0305200     -71555.000
    239.720      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
NH4CLO4(I)        Ammonium Perchlorate. Chase,1998 p766.                  React.
 1 j12/62 N   1.00H   4.00CL  1.00O   4.00    0.00 1  117.4890600    -295767.000
    100.000    513.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25238.000
-3.075344900D+03-2.136506130D+02 1.021583093D+01 1.659463617D-02 1.665266832D-05
-2.306096672D-08 1.543657693D-11                -3.825767260D+04-4.230254380D+01
NH4CLO4(II)       Ammonium Perchlorate. Chase,1998 p766.                  React.
 2 j12/62 N   1.00H   4.00CL  1.00O   4.00    0.00 2  117.4890600    -295767.000
    513.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25238.000
 9.739327490D+06-7.095035120D+04 2.133435041D+02-2.657628679D-01 2.034168863D-04
-5.628229760D-08 0.000000000D+00                3.485366440D+05-1.304962218D+03
   1000.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25238.000
 4.174684580D+06-1.716642636D+04 1.925955165D+01 3.499518910D-02-6.264443390D-06
-1.494354361D-09 0.000000000D+00                7.134752510D+04-1.274562074D+02
NH4NO3(IV)        Rhombic(IV). Gurvich,1989 pt1 p370 pt2 p322.            React.
 2 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 1   80.0433600    -365600.000
    256.200    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
-1.046561904D+07 1.560375249D+05-9.143153600D+02 2.670225944D+00-3.549932910D-03
 1.692615192D-06 0.000000000D+00               -7.861735160D+05 5.038726210D+03
    298.150    305.3807 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 5.865649329D+00 3.643028874D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.733937230D+04-2.614362444D+01
NH4NO3(III)       Rhombic(III). Gurvich,1989 pt1 p370 pt2 p322.           React.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 2   80.0433600    -365600.000
    305.380    357.2507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 7.233138213D+00 2.333270391D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.694179380D+04-2.929851693D+01
NH4NO3(II)        Tetragonal(II). Gurvich,1989 pt1 p370 pt2 p322.         React.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 3   80.0433600    -365600.000
    357.250    399.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 6.023205216D+01-1.767993544D-01 0.000000000D+00
 4.528829721D-07 0.000000000D+00               -5.478633510D+04-2.757806209D+02
NH4NO3(I)         Cubic(I). Gurvich,1989 pt1 p370 pt2 p322.               React.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 4   80.0433600    -365600.000
    399.000    442.8507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 1.295325882D+01 1.563531705D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.783701280D+04-5.848510823D+01
NH4NO3(L)         Liquid  Gurvich,1989 pt1 p370 pt2 p322.                 React.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 5   80.0433600    -365600.000
    442.850    900.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 1.936373881D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.843793300D+04-8.903005276D+01
N2(L)             Nitrogen. McBride,1996 pp85,93.
 0 g 6/96 N   2.00    0.00    0.00    0.00    0.00 1   28.0134000     -12107.000
     77.352      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0            0.000
N2H4(L)           Hydrazine.Hf:Gurvich,1989 pt1 p360. Chase,1998(12/65).  React.
 1 g11/99 N   2.00H   4.00    0.00    0.00    0.00 1   32.0451600     50380.000
    100.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 2.080965738D+04-7.418167630D+02 1.916569184D+01-4.539330120D-02 1.342024252D-04
-1.470873931D-07 6.056288260D-11                5.735408180D+03-8.820213940D+01
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N2O4(L)            Dinitrogen tetroxide. McBride,1996 pp85,93.
 0 g 6/96 N   2.00O    4.00     0.00     0.00     0.00 1    92.0110000      -17549.000
    298.150       0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
O2(L)              Oxygen. McBride,1996 pp85,93.
 0 g 6/96 O   2.00     0.00     0.00     0.00     0.00 1    31.9988000      -12979.000
     90.170       0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
O3(L)              Ozone. McBride,1996 pp85,93.
 0 g 6/96 O   3.00     0.00     0.00     0.00     0.00 1    47.9982000      122527.000
    161.850       0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
RP-1               Mehta et.al. AIAA 95-2962 1995. Hcomb(high) = 19923.BTU/#
 0 gll/00 C   1.00H    1.95     0.00     0.00     0.00 1    13.9761830      -24717.700
    298.150       0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0              0.000
END REACTANTS
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13. ABSTRACT ***(Maximum 200 words)***

This report documents the library of thermodynamic data used with the NASA Glenn computer program CEA (Chemical Equilibrium with Applications). This library, containing data for over 2000 solid, liquid, and gaseous chemical species for temperatures ranging from 200 to 20 000 K, is available for use with other computer codes as well. The data are expressed as least-squares coefficients to a seven-term functional form for $C_p^o(T)/R$ with integration constants for $H^o(T)/RT$ and $S^o(T)/R$. The NASA Glenn computer program PAC (Properties and Coefficients) was used to calculate thermodynamic functions and to generate the least-squares coefficients. PAC input was taken from a variety of sources. A complete listing of the database is given along with a summary of thermodynamic properties at 0 and 298.15 K.

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